Toward improved OHC mapping and uncertainty quantification by modeling vertical spatio-temporal dependence

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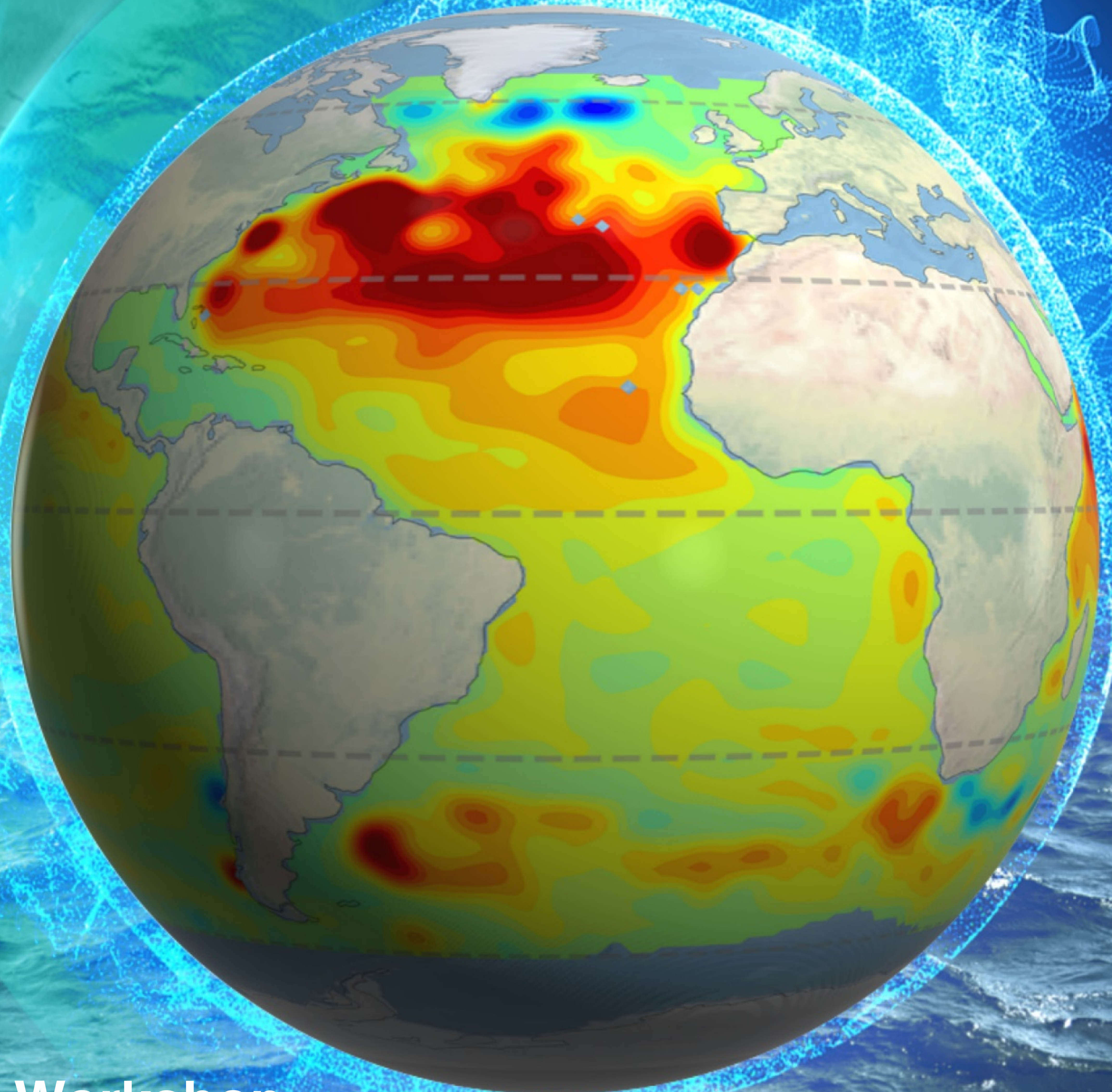
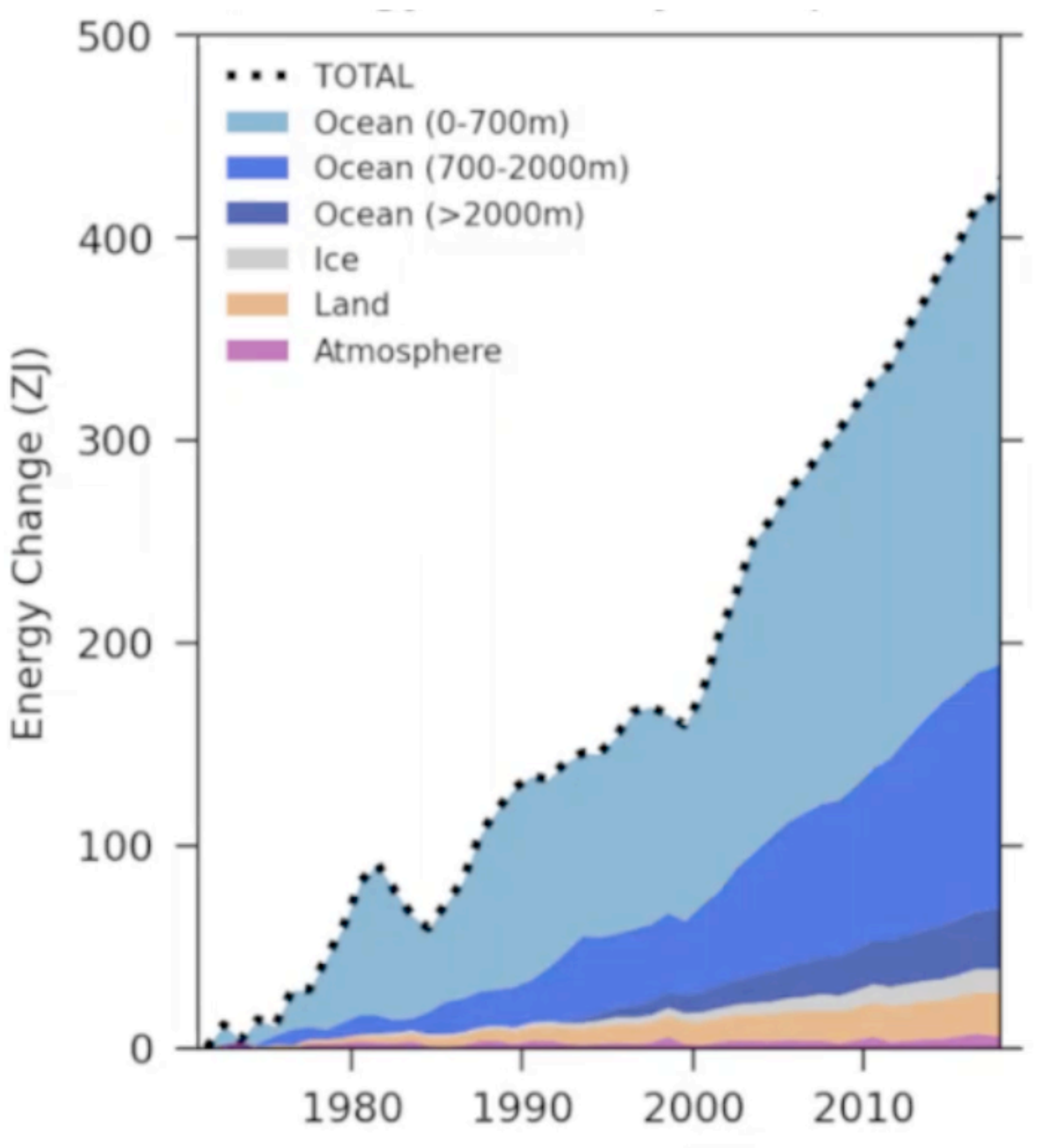


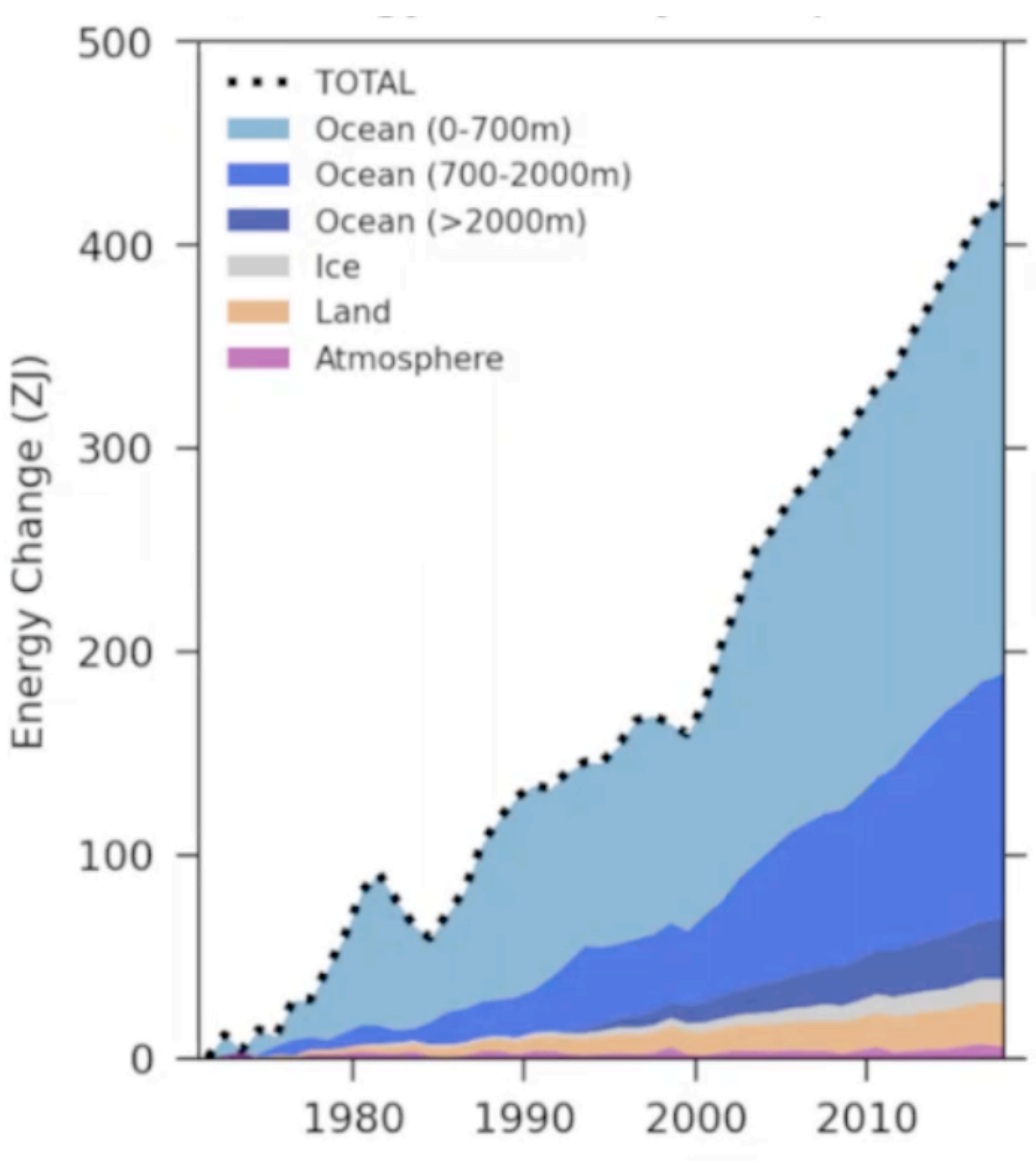
Earth Energy Imbalance Assessment Workshop, 15-17 May 2023, Hosted as a Hybrid Event at ESA-ESRIN, Frascati (Rome), Italy

Most of the excess heat in the climate system has been stored in the ocean



(IPCC 2021)

Changes in OHC contribute to extreme climate events

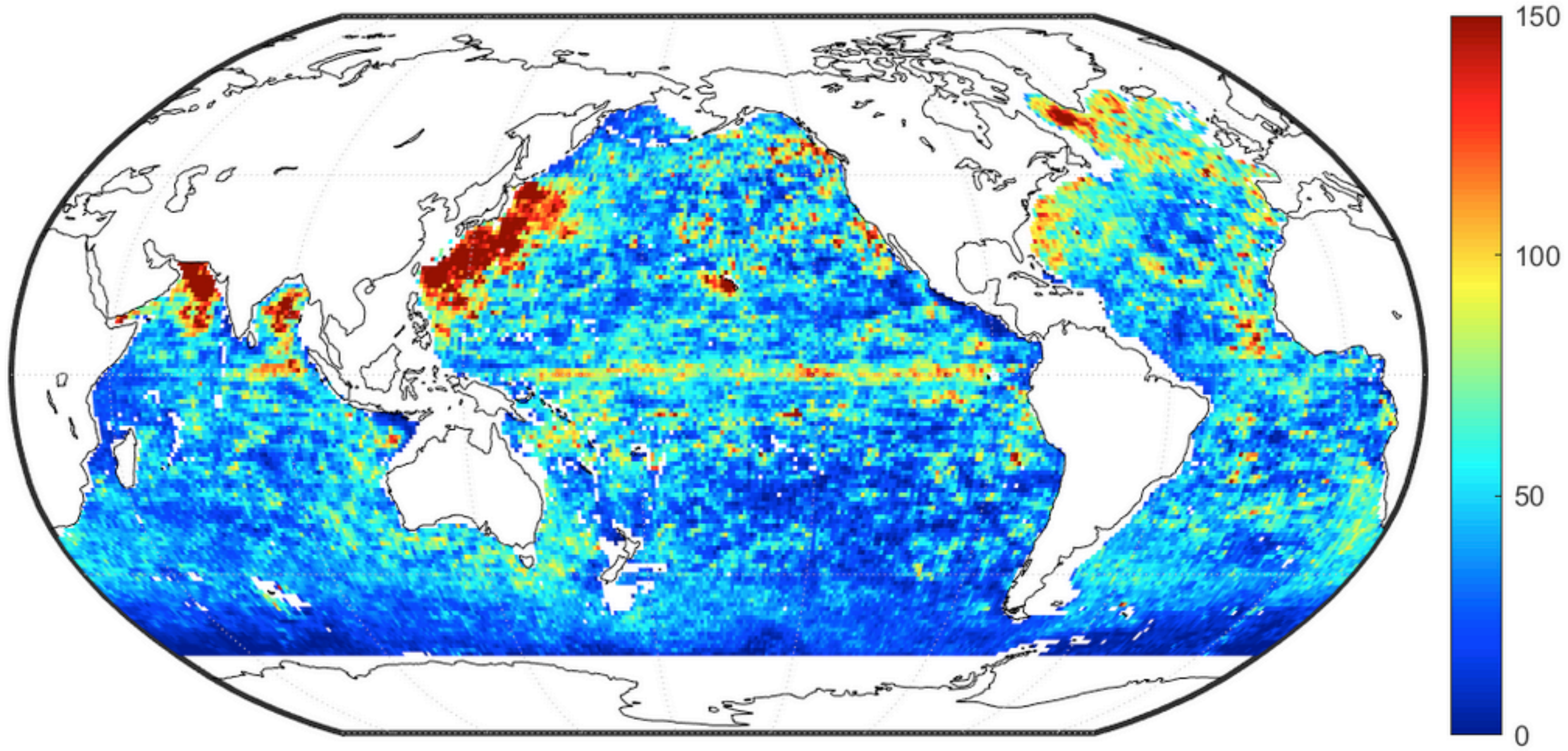


(IPCC 2021)

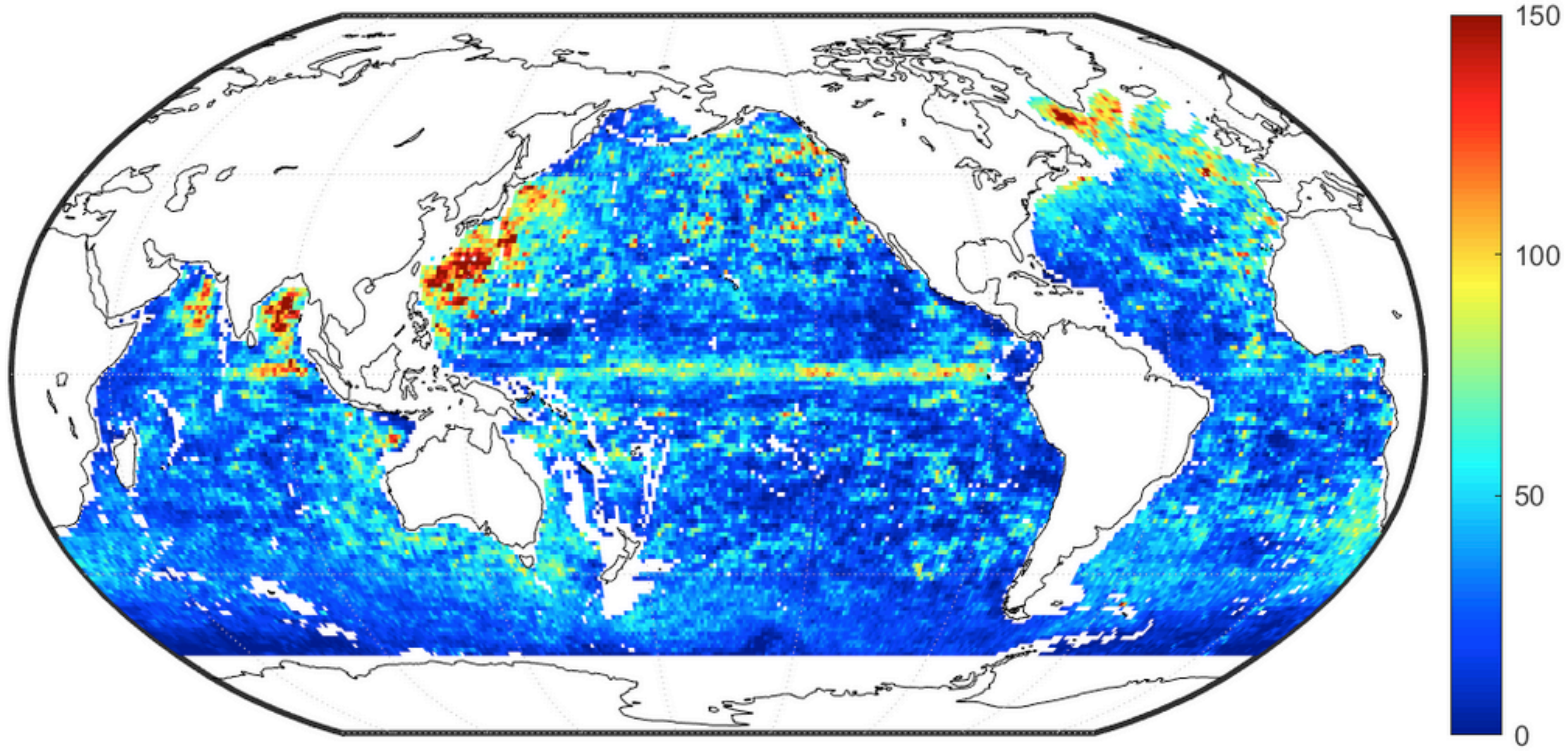
Intensified tropical storms

Rising sea levels

We use Argo data (2004-2021) to estimate 15-1850 dbar OHC

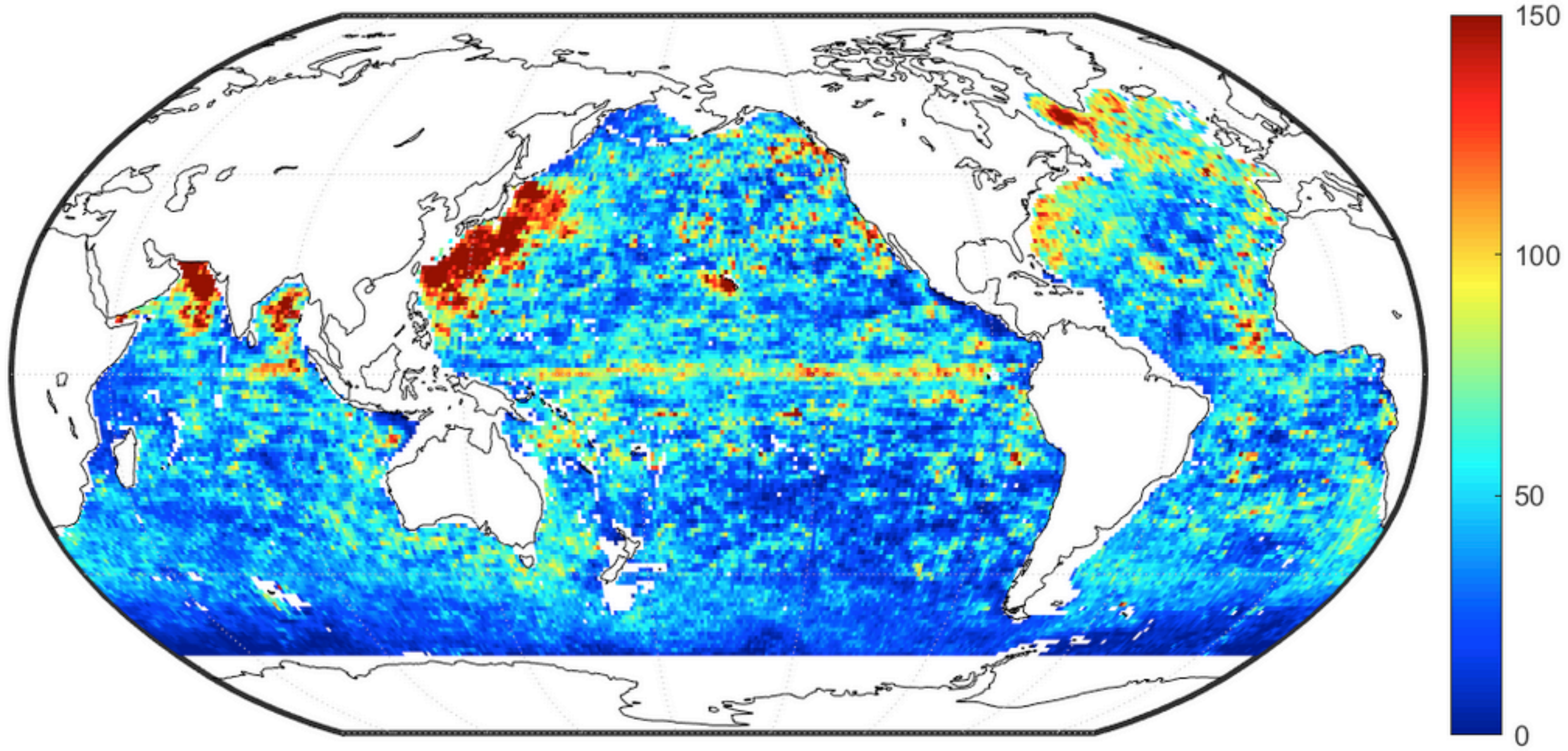


Top layer profiles (15-975 dbar)

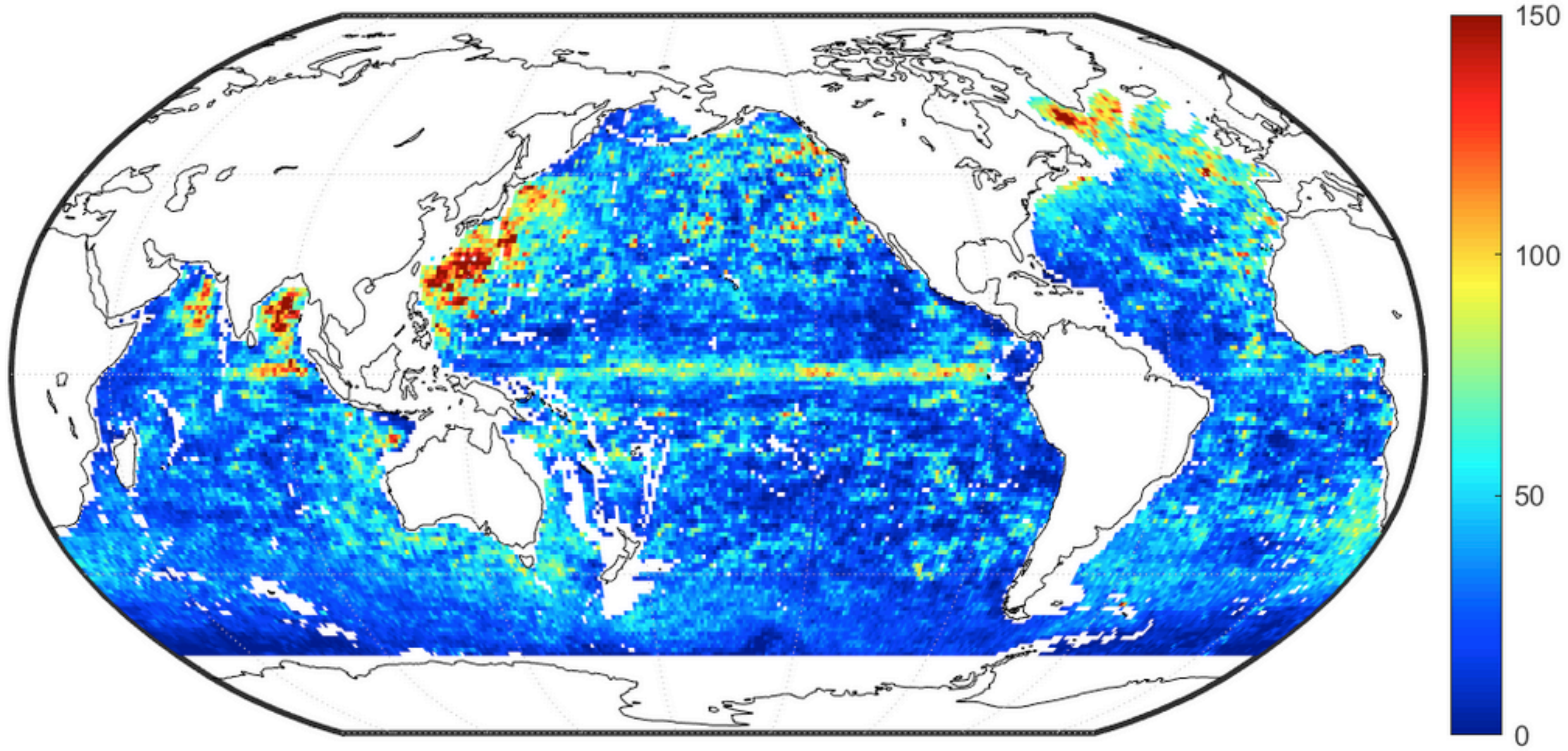


Bottom layer profiles (975-1850 dbar)

We use Argo data (2004-2021) to estimate 15-1850 dbar OHC



→ **Top layer profiles (15-975 dbar)**



→ **Bottom layer profiles (975-1850 dbar)**

Due to having fewer observations deeper in the water column, we model the OHC in the top and bottom layers **separately.**

How do we model OHC from sparse observations?

1. Model the **vertical dimension** (consider two layers and integrate Argo profiles in each layer)

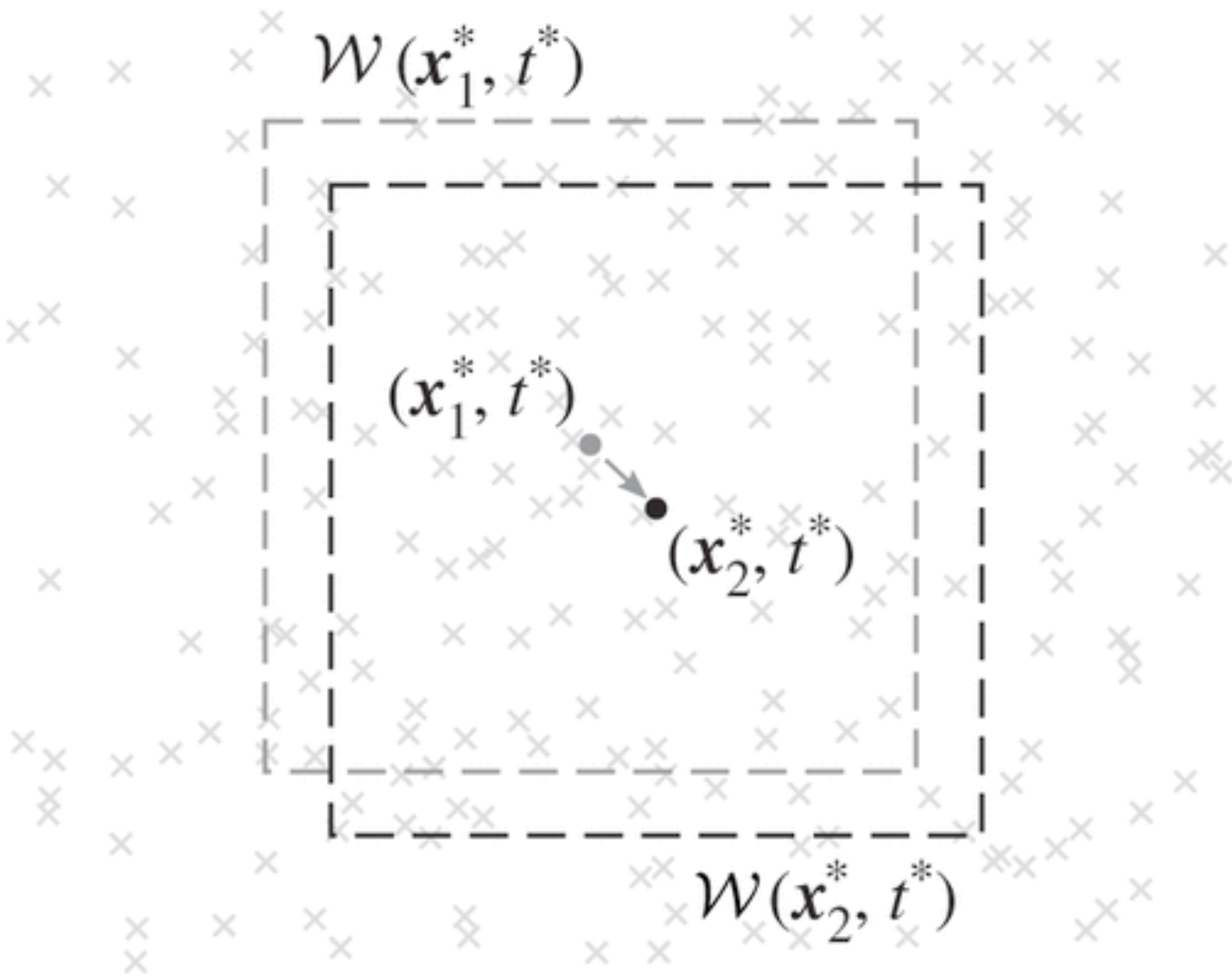
2. Model **horizontal and temporal dimension**

3. Estimate **uncertainties** based on (1) and (2)

We can estimate a gridded temperature field with GP regression

1. Model temperature mean field: local least squares regression (Roemmich and Gilson 2009) + linear time trend

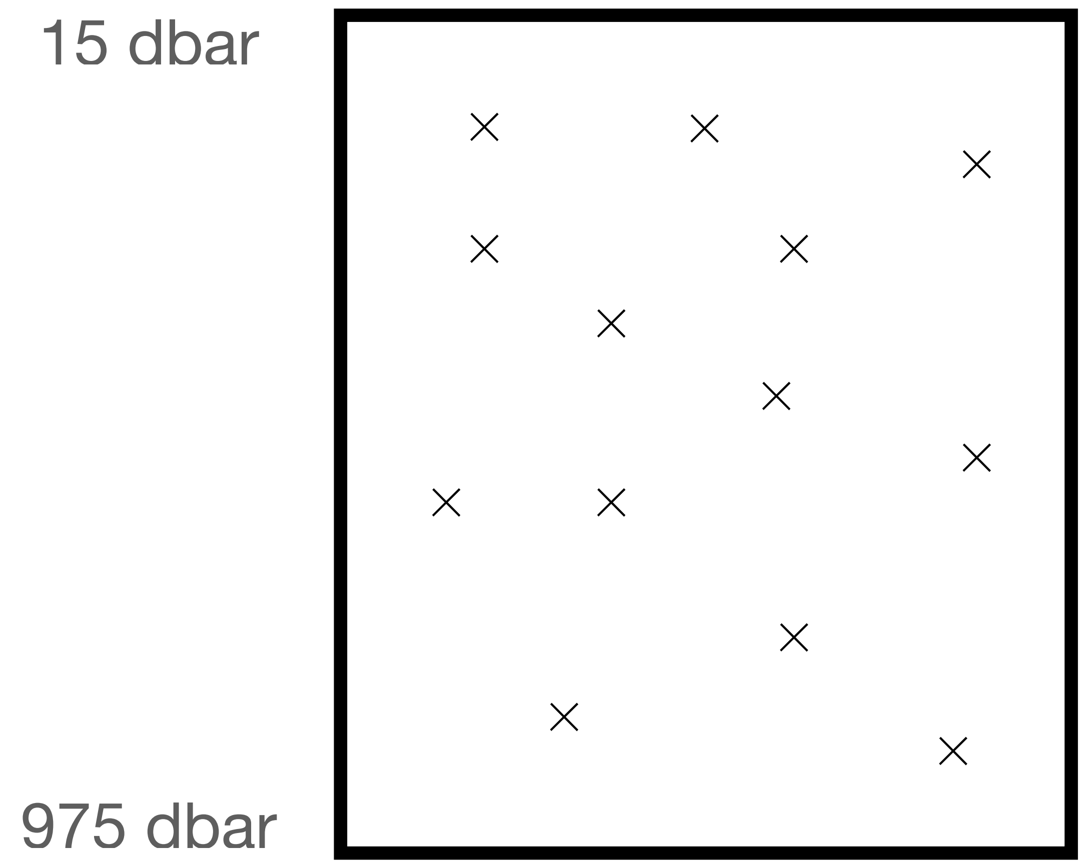
2. Model residuals **(anomalies)**: **locally stationary** Gaussian process (GP) regression (Kuusela and Stein 2018)



How do we estimate uncertainties for the total (top + bottom layers) OHC?

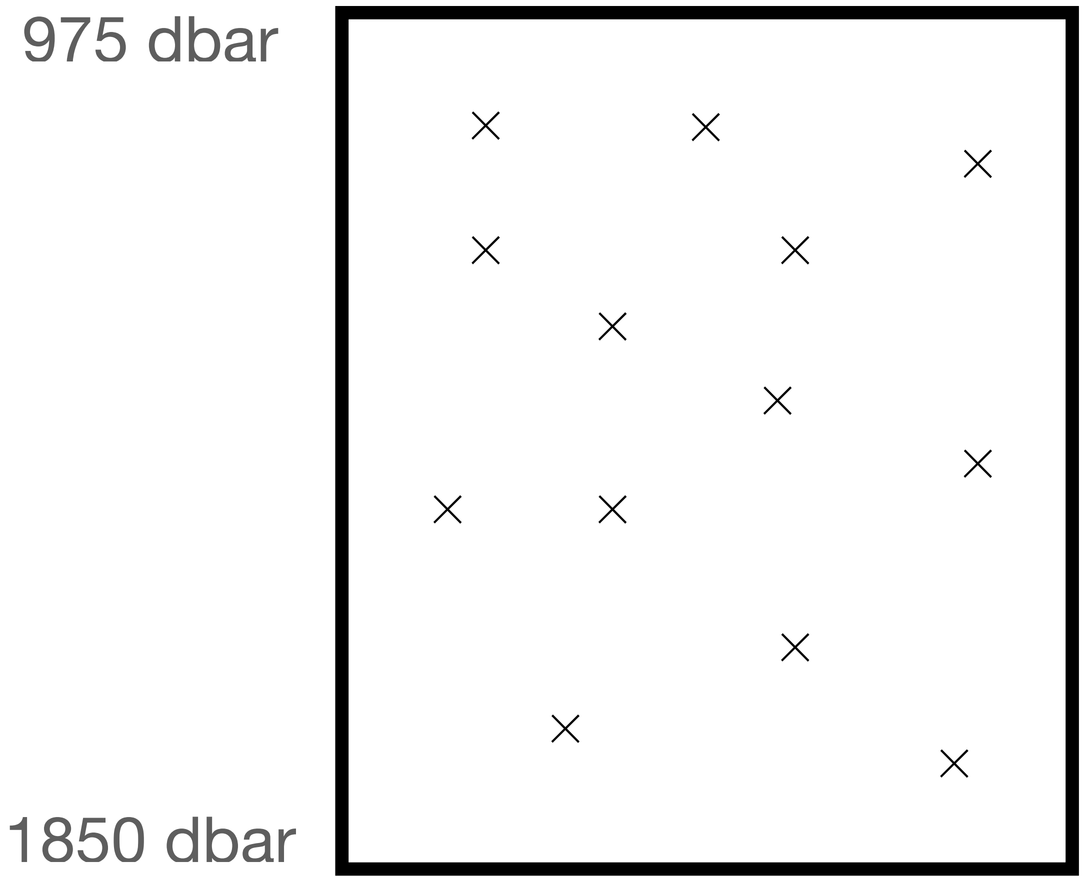
$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$$

How do we estimate uncertainties for the total (top + bottom layers) OHC?



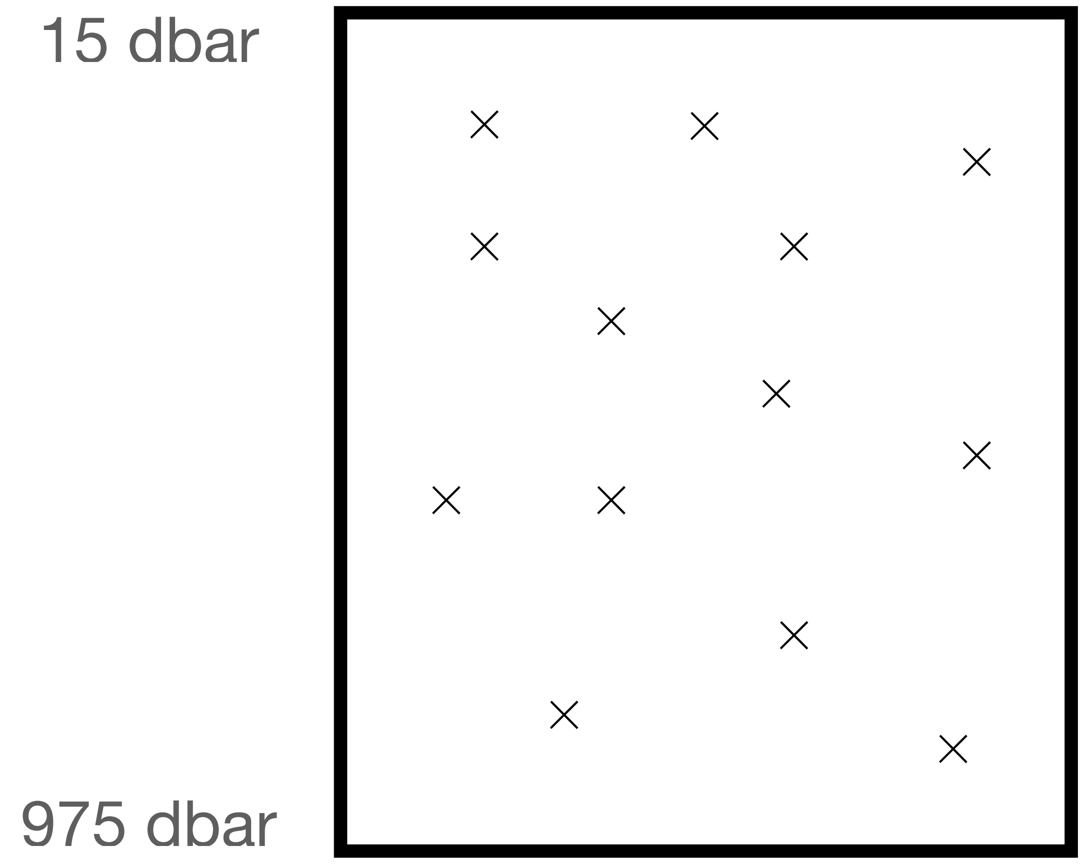
$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})$$

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$$

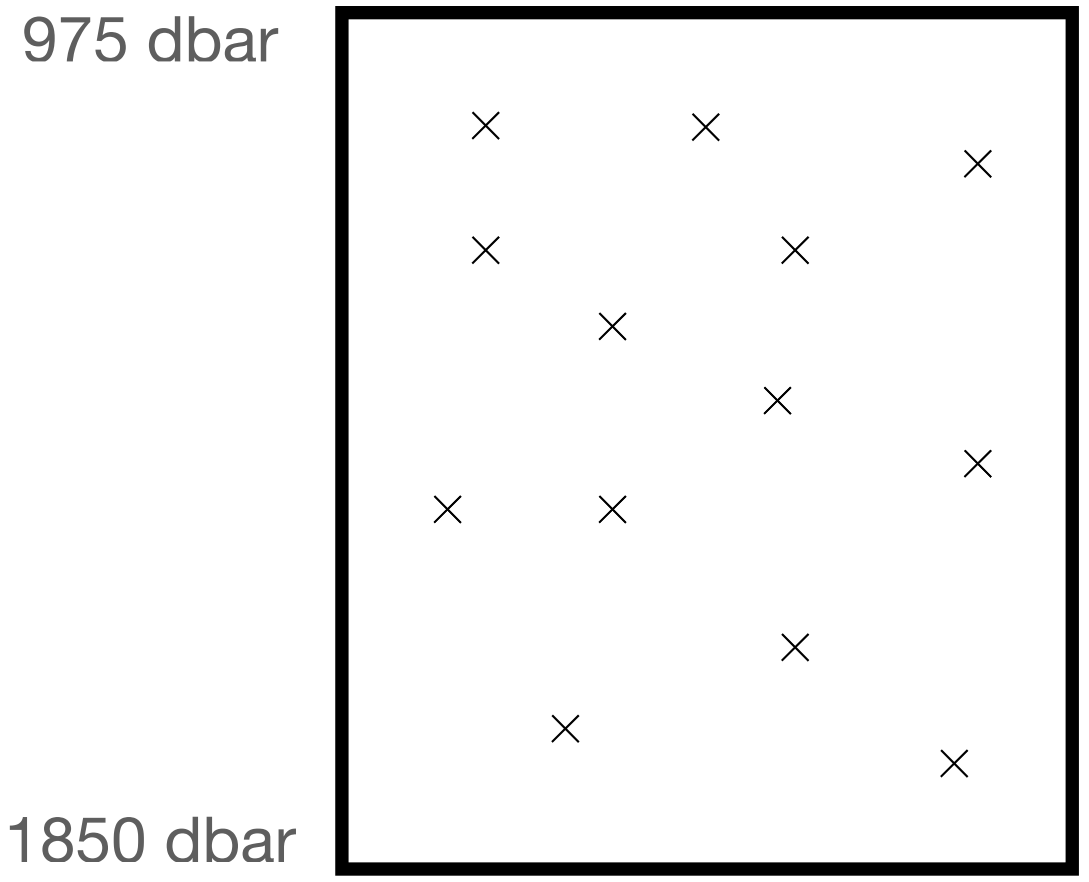


$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

How do we estimate uncertainties for the total (top + bottom layers) OHC?



$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})$$



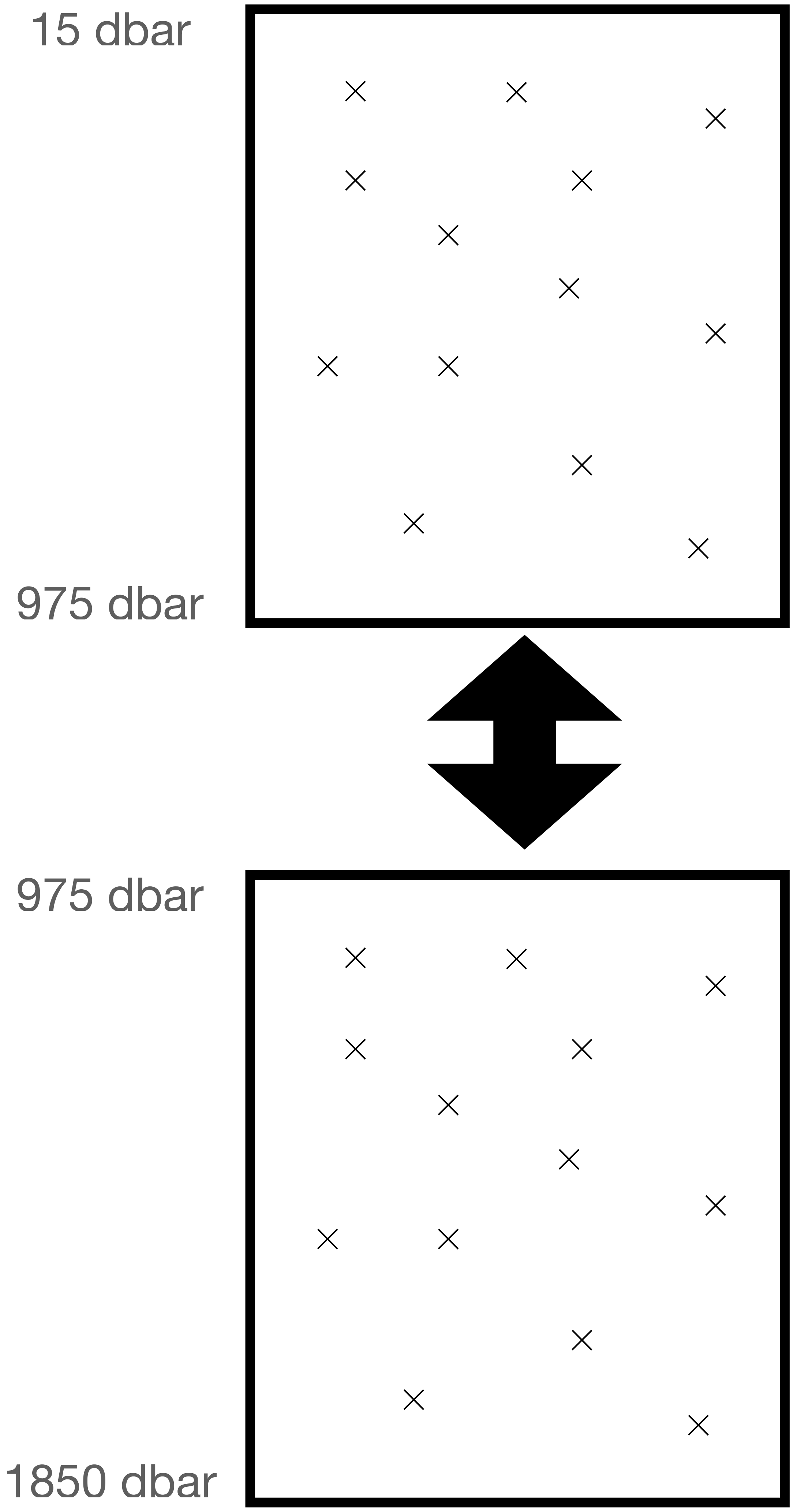
$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

$$\mathrm{Var}(\cancel{\mathrm{OHC}_{\mathrm{total}}}|\mathrm{data})$$

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data}) + \mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

Summing the variances for each layer **underestimates** the uncertainties of the total OHC.

How do we estimate uncertainties for the total (top + bottom layers) OHC?

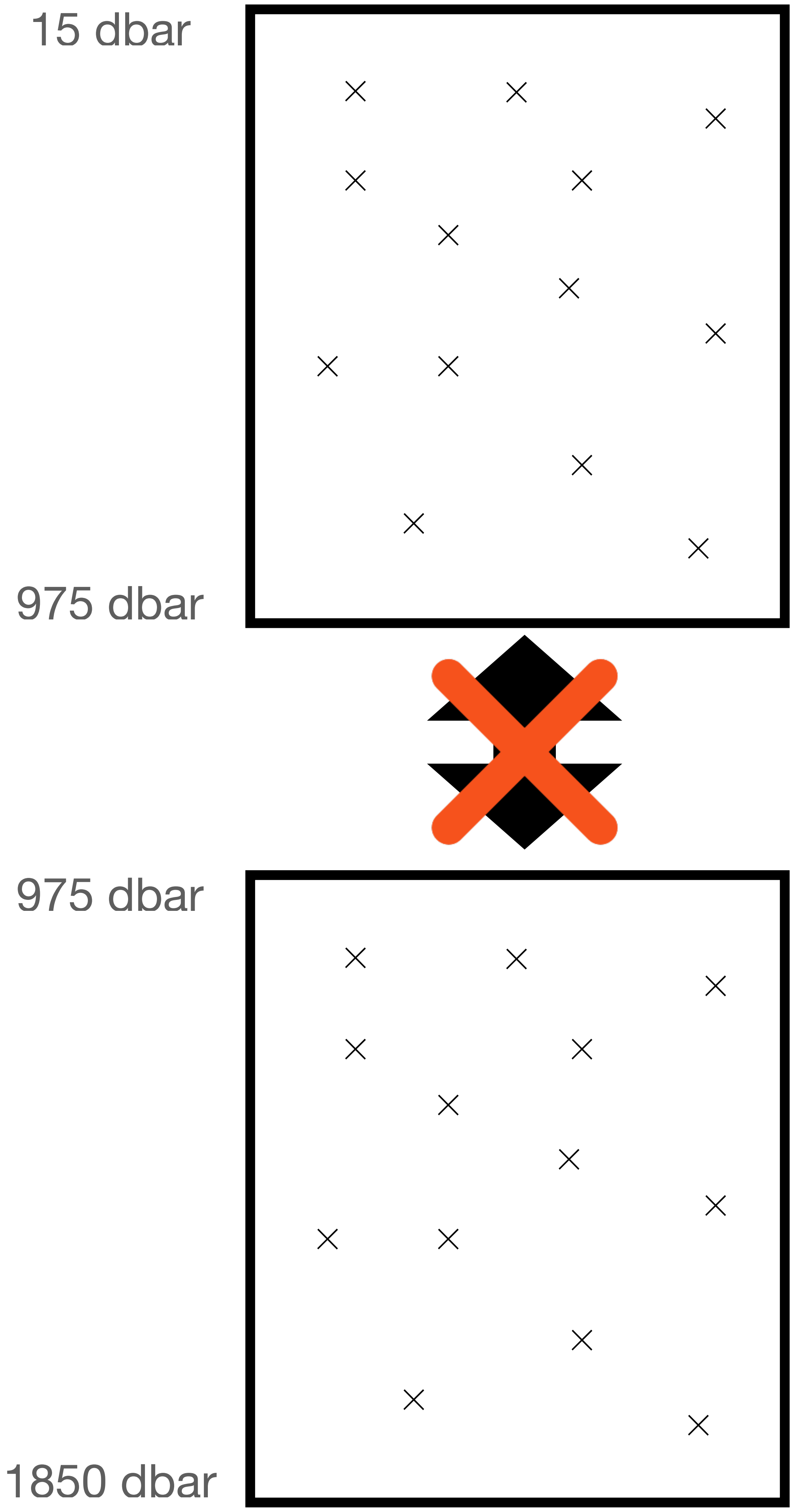


$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})$$

$$2\mathrm{Cov}(\mathrm{OHC}_{\mathrm{top}}, \mathrm{OHC}_{\mathrm{bot}}|\mathrm{data}) \longrightarrow \mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$$

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

How do we estimate uncertainties for the total (top + bottom layers) OHC?



$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})$$

$$2\mathrm{Cov}(\mathrm{OHC}_{\mathrm{top}}, \mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$$

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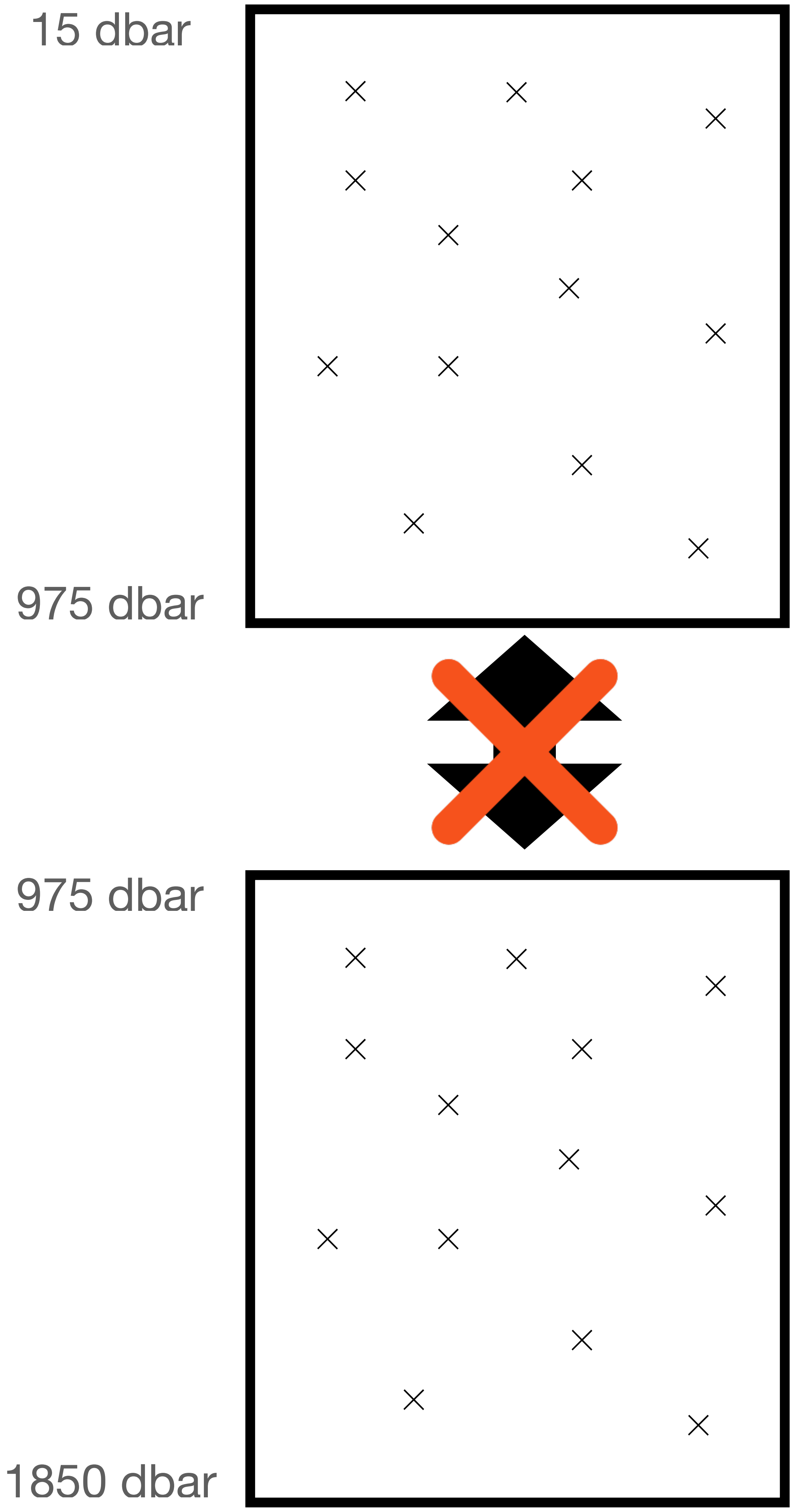


$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})$$

$$2\mathrm{Cov}(\mathrm{OHC}_{\mathrm{top}}, \mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$$

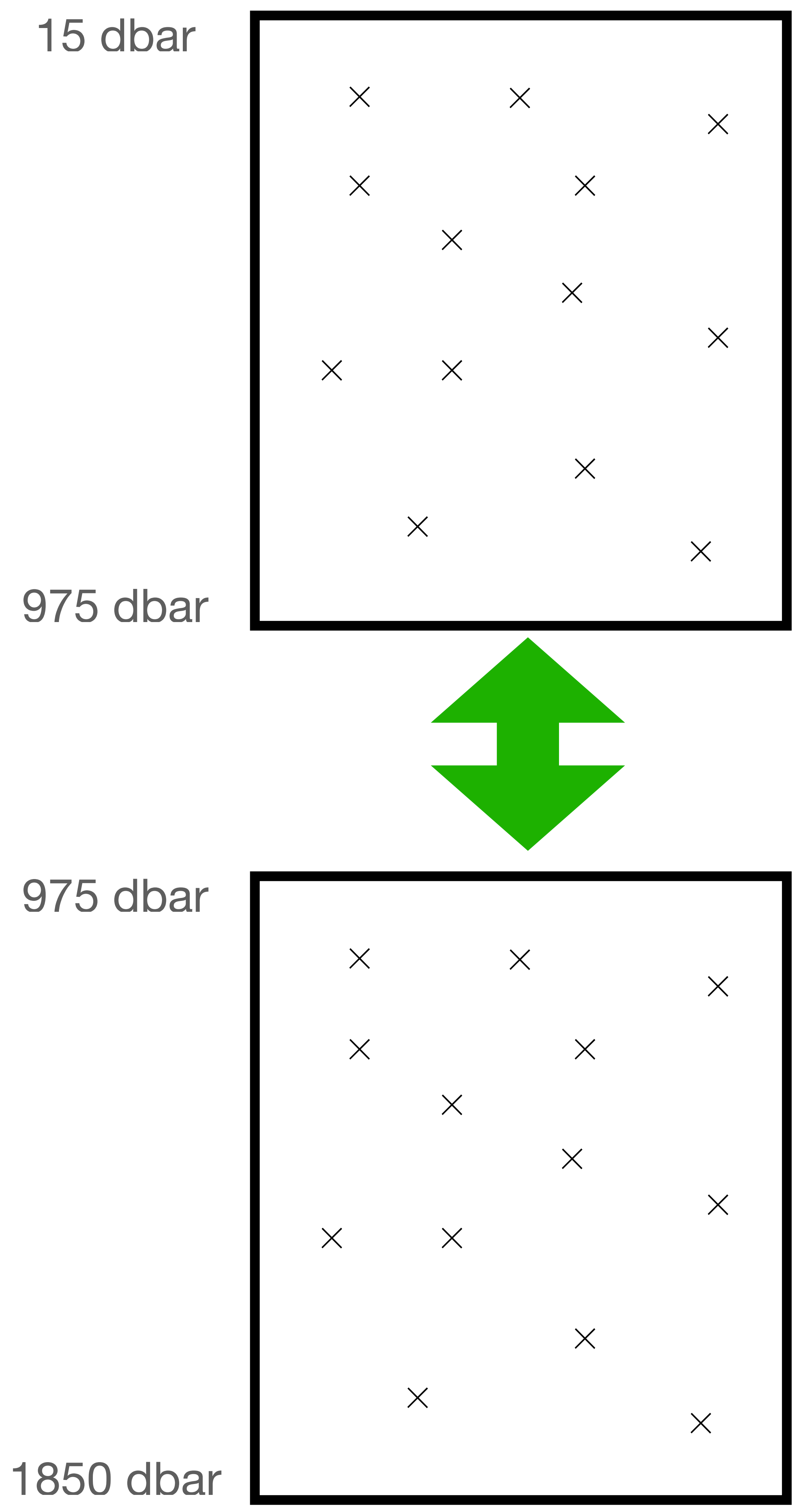
$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$$

(conservative upper bound)

$$(\sqrt{\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})} + \sqrt{\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})})^2$$

Squaring the sum of the standard deviations for each layer **overestimates** the uncertainties of the total OHC.

How do we estimate uncertainties for the total (top + bottom layers) OHC?



$\mathrm{Var}(\mathrm{OHC}_{\mathrm{top}}|\mathrm{data})$

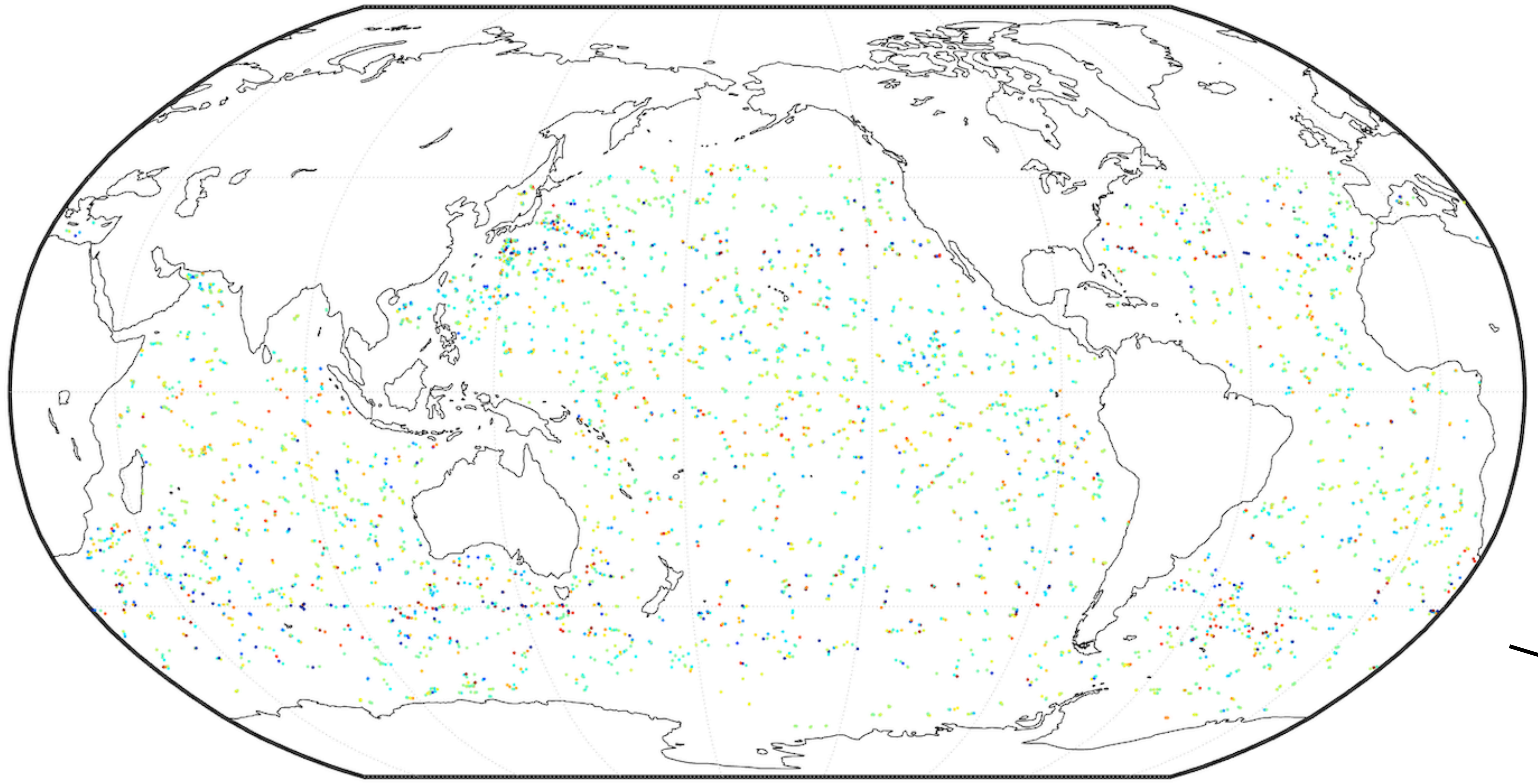
$2\mathrm{Cov}(\mathrm{OHC}_{\mathrm{top}}, \mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$

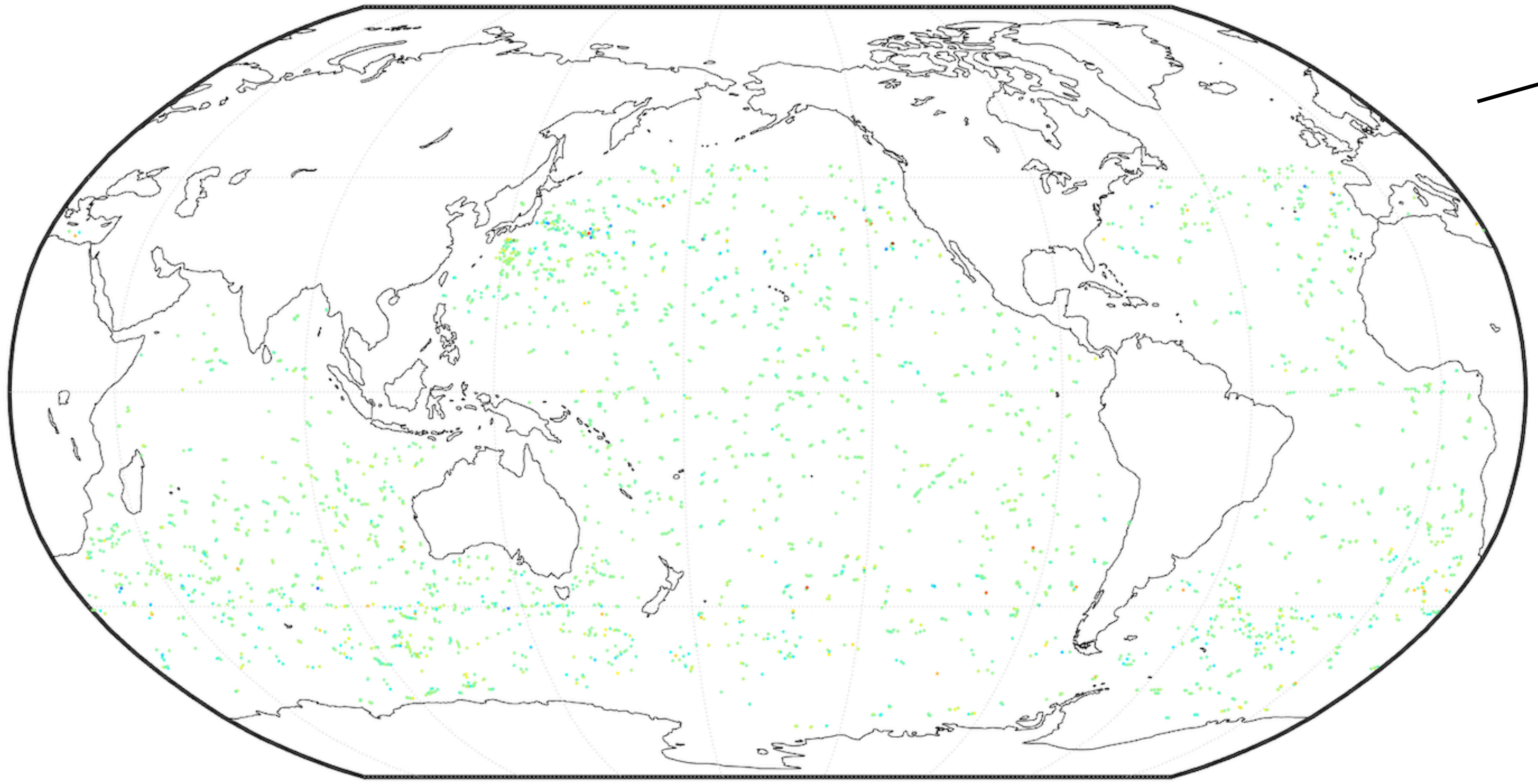
$\mathrm{Var}(\mathrm{OHC}_{\mathrm{bot}}|\mathrm{data})$

$\mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$

We can improve the uncertainty estimates by also modeling the **correlation**.

A bivariate GP model accounts for cross-layer correlation

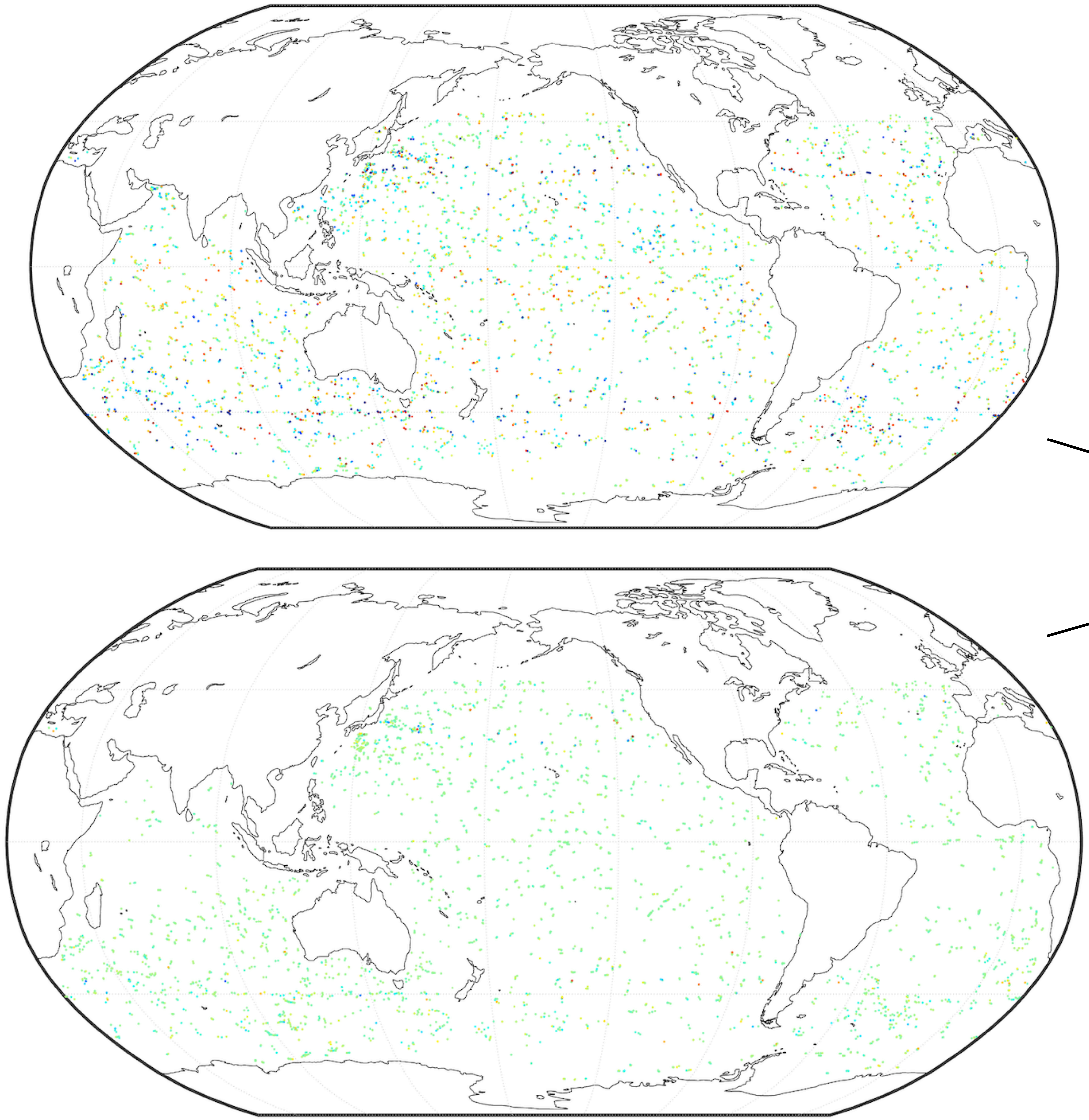




Temperature residuals

$$\begin{bmatrix} y_{\text{top}} \\ y_{\text{bot}} \end{bmatrix}_{i,j}$$

A bivariate GP model accounts for cross-layer correlation

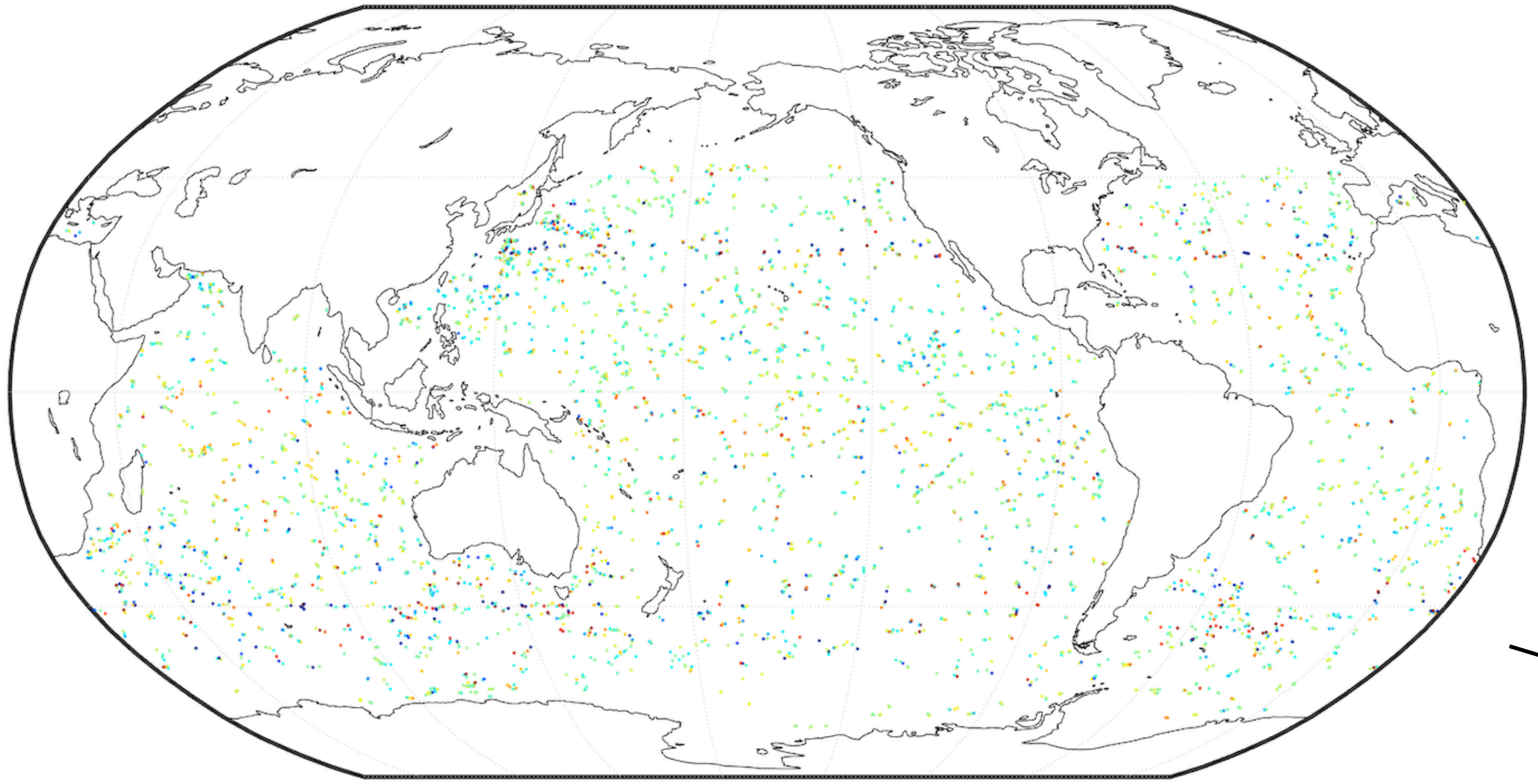


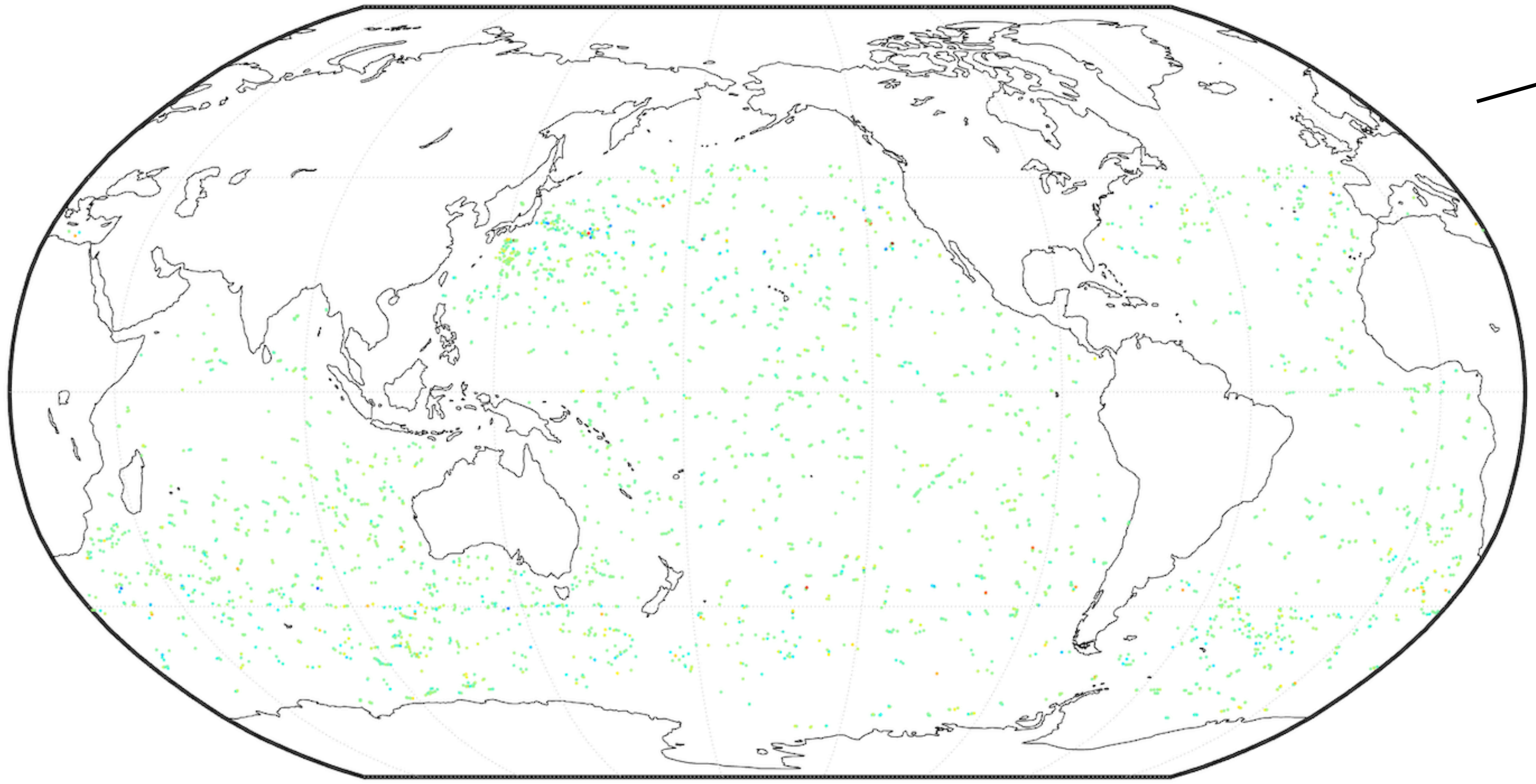
Temperature residuals   **Latitude Longitude**   **Date**

$$\begin{bmatrix} y_{\text{top}} \\ y_{\text{bot}} \end{bmatrix}_{i,j} = f_i\left(\begin{bmatrix} x_{\text{top}} \\ x_{\text{bot}} \end{bmatrix}_{i,j}, \begin{bmatrix} t_{\text{top}} \\ t_{\text{bot}} \end{bmatrix}_{i,j}\right)$$

$$f_i \overset{\text{iid}}{\sim} \text{GP}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{K}(x_1, t_1, x_2, t_2; \boldsymbol{\theta})\right)$$

A bivariate GP model accounts for cross-layer correlation





Temperature residuals | **Latitude Longitude** | **Date** | **Nugget effect**

$$\begin{bmatrix} y_{\text{top}} \\ y_{\text{bot}} \end{bmatrix}_{i,j} = f_i\left(\begin{bmatrix} x_{\text{top}} \\ x_{\text{bot}} \end{bmatrix}_{i,j}, \begin{bmatrix} t_{\text{top}} \\ t_{\text{bot}} \end{bmatrix}_{i,j}\right) + \begin{bmatrix} \epsilon_{\text{top}} \\ \epsilon_{\text{bot}} \end{bmatrix}_{i,j}$$

$$f_i \overset{\text{iid}}{\sim} \text{GP}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{K}(x_1, t_1, x_2, t_2; \boldsymbol{\theta})\right)$$

$$\begin{bmatrix} \epsilon_{\text{top}} \\ \epsilon_{\text{bot}} \end{bmatrix} \overset{\text{iid}}{\sim} \text{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\boldsymbol{\theta}_{\boldsymbol{\epsilon}})\right)$$

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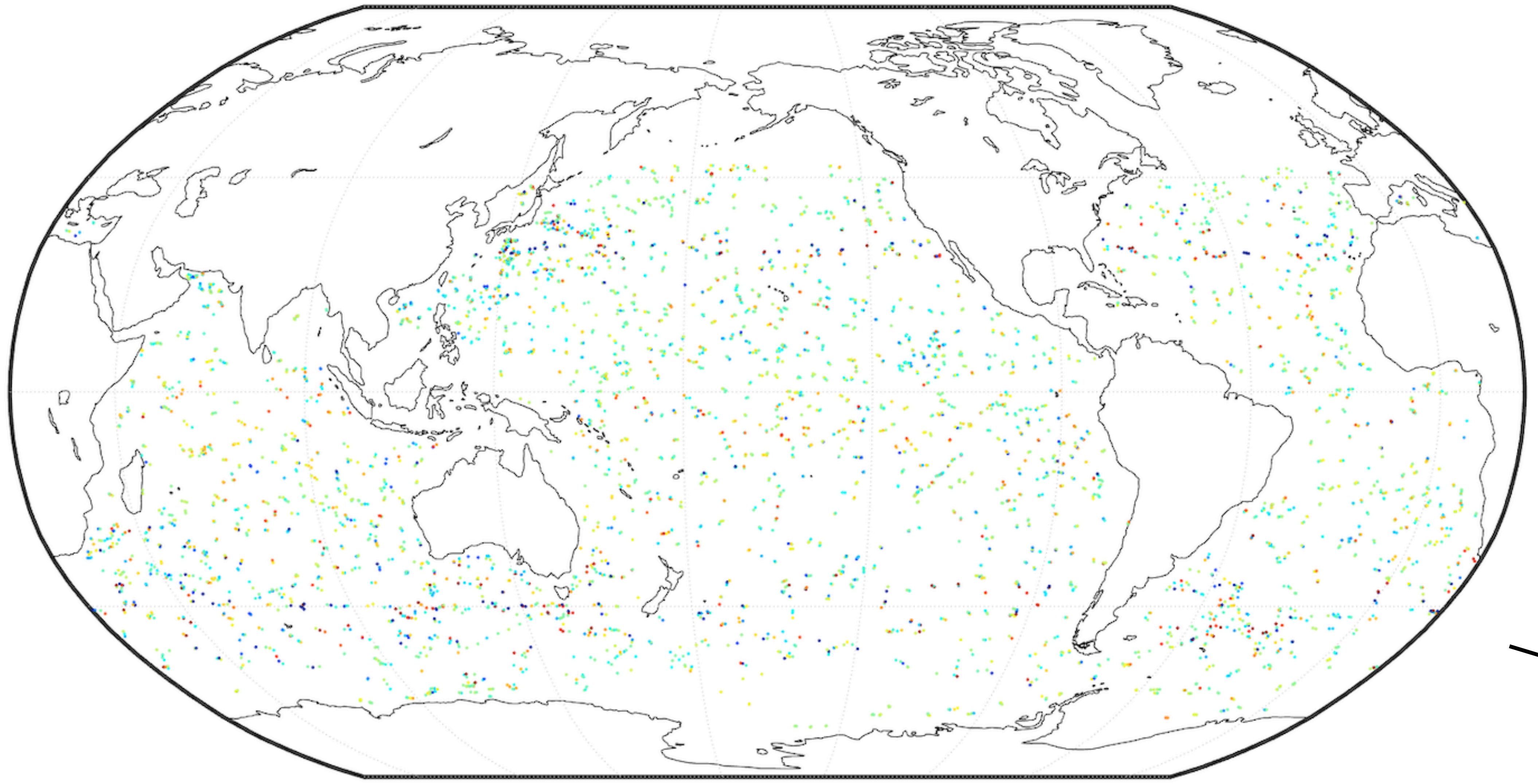

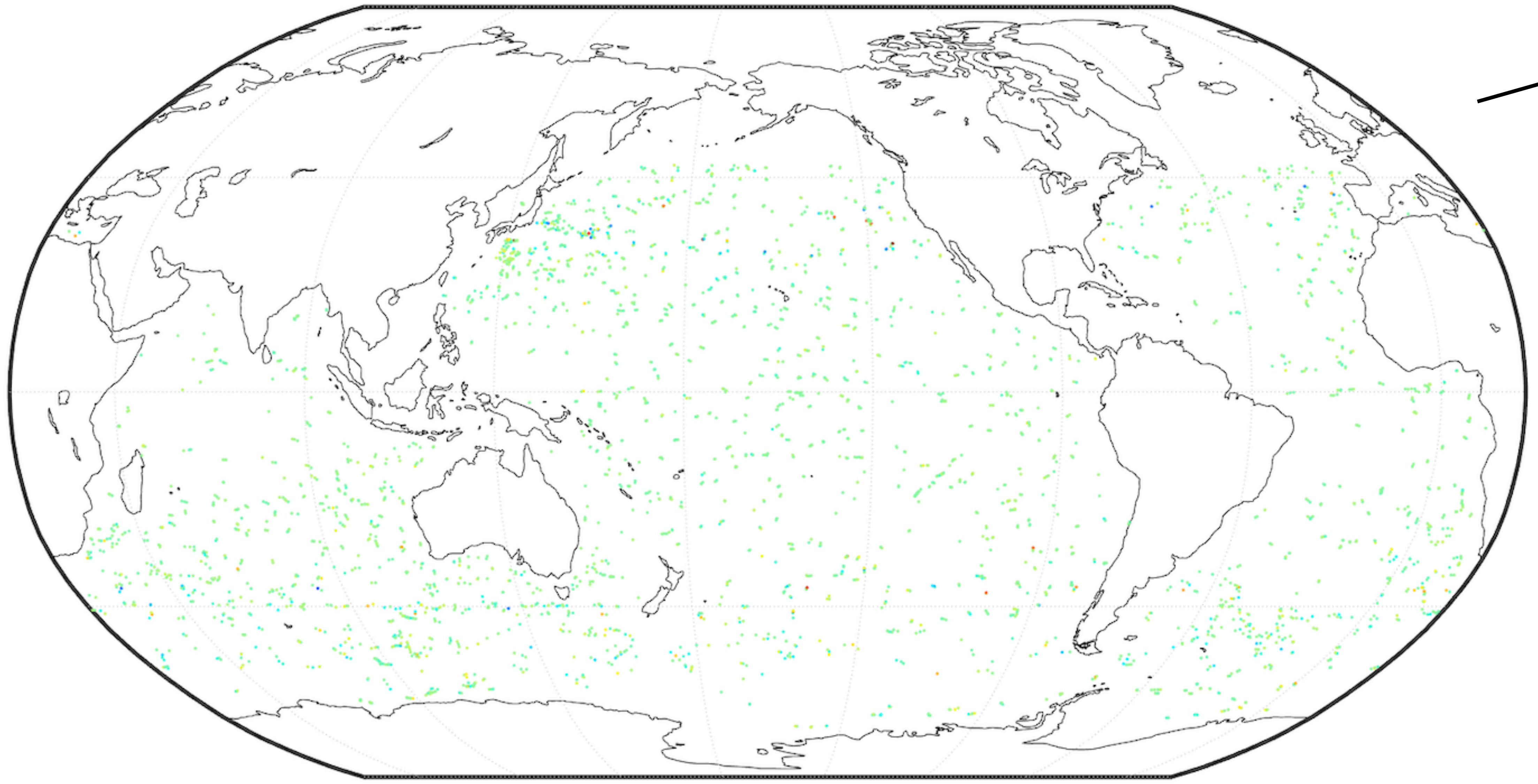

Temperature residuals | Latitude Longitude | Date | Nugget effect

$$\begin{bmatrix} y_{\text{top}} \\ y_{\text{bot}} \end{bmatrix}_{i,j} = f_i\left(\begin{bmatrix} x_{\text{top}} \\ x_{\text{bot}} \end{bmatrix}_{i,j}, \begin{bmatrix} t_{\text{top}} \\ t_{\text{bot}} \end{bmatrix}_{i,j}\right) + \begin{bmatrix} \epsilon_{\text{top}} \\ \epsilon_{\text{bot}} \end{bmatrix}_{i,j}$$

$$f_i \overset{\text{iid}}{\sim} \mathrm{GP}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{K}(x_1, t_1, x_2, t_2; \boldsymbol{\theta})\right)$$

(Covariance function)

$$\begin{bmatrix} \epsilon_{\text{top}} \\ \epsilon_{\text{bot}} \end{bmatrix} \overset{\text{iid}}{\sim} \mathrm{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \boldsymbol{\Sigma}_\epsilon(\boldsymbol{\theta}_\epsilon)\right)$$

A bivariate GP model accounts for cross-layer correlation

Marginal covariance
(Kuusela and Stein 2018)

$$\boldsymbol{K}_{\mathrm{ii}}(\boldsymbol{z_1}, \boldsymbol{z_2}; \boldsymbol{\theta})$$

A bivariate GP model accounts for cross-layer correlation

Marginal covariance
(Kuusela and Stein 2018)

$$\boldsymbol{K}_{\mathrm{ii}}(\boldsymbol{z_1}, \boldsymbol{z_2}; \boldsymbol{\theta}) = \frac{\delta_i^2}{\sqrt{|\boldsymbol{\Theta}_i|}}$$

GP variance

A bivariate GP model accounts for cross-layer correlation

Marginal covariance
(Kuusela and Stein 2018)

$$\boldsymbol{K}_{\mathrm{ii}}(\boldsymbol{z_1}, \boldsymbol{z_2}; \boldsymbol{\theta}) = \frac{\delta_i^2}{\sqrt{|\boldsymbol{\Theta}_i|}} \exp(-\sqrt{(\boldsymbol{z_1} - \boldsymbol{z_2})^{\mathrm{T}} \boldsymbol{\Theta}_i^{-1} (\boldsymbol{z_1} - \boldsymbol{z_2})})$$

GP variance

Space-time distance w/ length scale parameters

A bivariate GP model accounts for cross-layer correlation

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(Kuusela and Stein 2018)

$$\boldsymbol{K}_{\mathrm{ii}}(\boldsymbol{z_1}, \boldsymbol{z_2}; \boldsymbol{\theta}) = \frac{\delta_i^2}{\sqrt{|\boldsymbol{\Theta}_i|}} \exp(-\sqrt{(\boldsymbol{z_1} - \boldsymbol{z_2})^{\mathrm{T}} \boldsymbol{\Theta}_i^{-1} (\boldsymbol{z_1} - \boldsymbol{z_2})})$$

GP variance

Space-time distance
w/ length scale parameters

Cross-covariance
(Kleiber and Nychka 2012)

$$\boldsymbol{K}_{\mathrm{top,bot}}(\boldsymbol{z_1}, \boldsymbol{z_2}; \boldsymbol{\theta}) = \beta \frac{\delta_{\mathrm{top}}\delta_{\mathrm{bot}}}{\sqrt{|\boldsymbol{\Theta}_{\mathrm{top,bot}}|}} \exp(-\sqrt{(\boldsymbol{z_1} - \boldsymbol{z_2})^{\mathrm{T}} \boldsymbol{\Theta}_{\mathrm{top,bot}}^{-1} (\boldsymbol{z_1} - \boldsymbol{z_2})})$$

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GP variance

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(Cross) correlation

Obtaining uncertainties is facilitated by local conditional simulations

$\text{anomaly}|\text{data}$?

Obtaining uncertainties is facilitated by local conditional simulations

$\text{anomaly}|\text{data}$ - **multivariate normal** with conditional covariance Σ_i

(parameterized by estimated GP variance, length scales, cross-correlation)

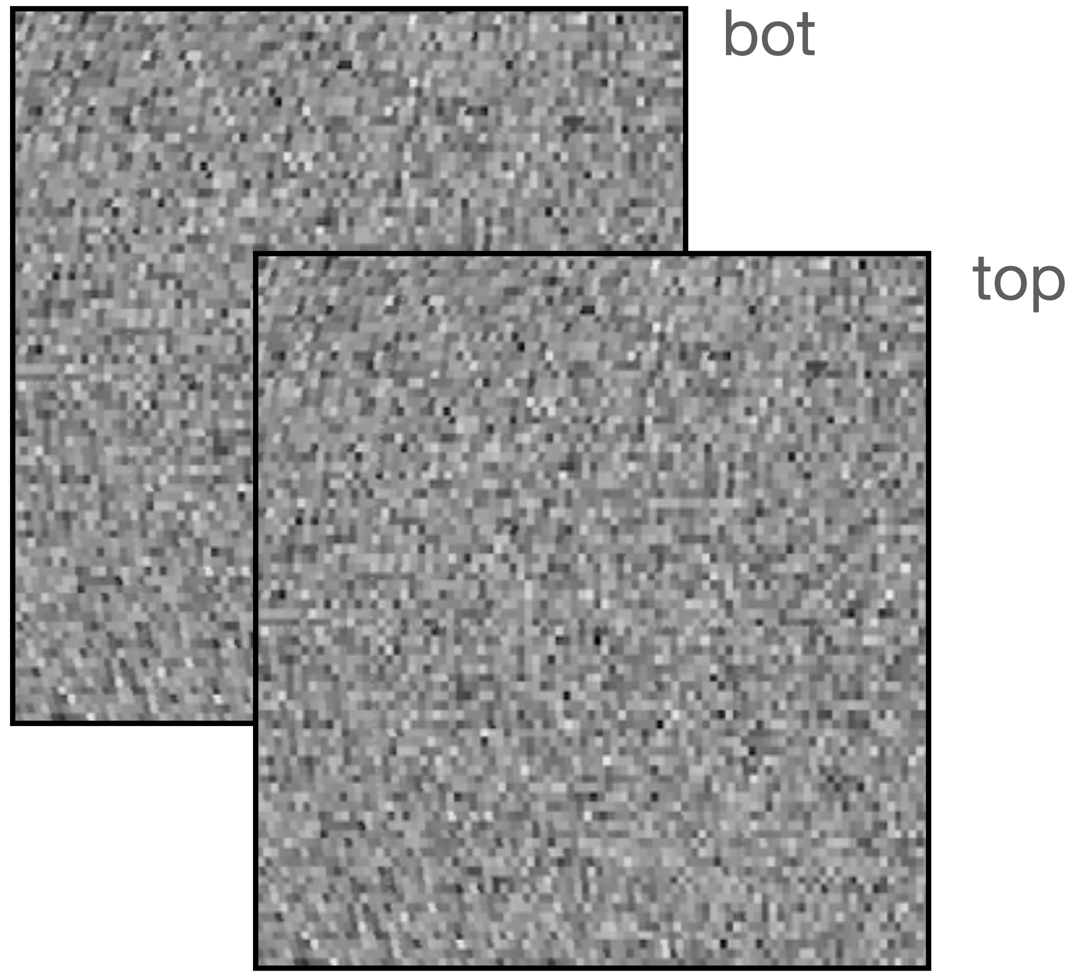
Obtaining uncertainties is facilitated by local conditional simulations

$\mathrm{anomaly}|\mathrm{data}$ - **multivariate normal** with conditional covariance $\boldsymbol{\Sigma}_i$

(parameterized by estimated GP variance, length scales, cross-correlation)

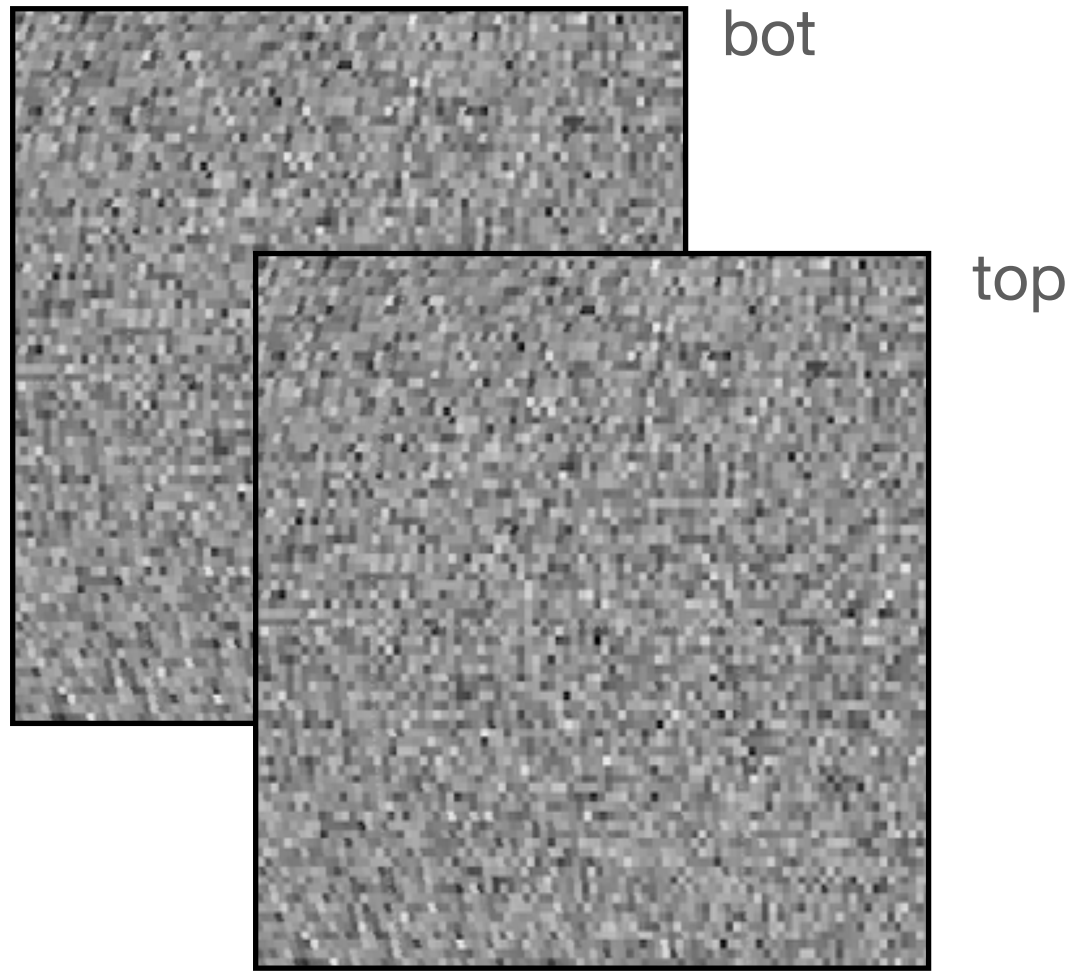
Local conditional simulations! (extension of Nychka et.al. 2018)

Obtaining uncertainties is facilitated by local conditional simulations



Simulate Gaussian
white noise over grid
(keep fixed)

Obtaining uncertainties is facilitated by local conditional simulations



Simulate Gaussian
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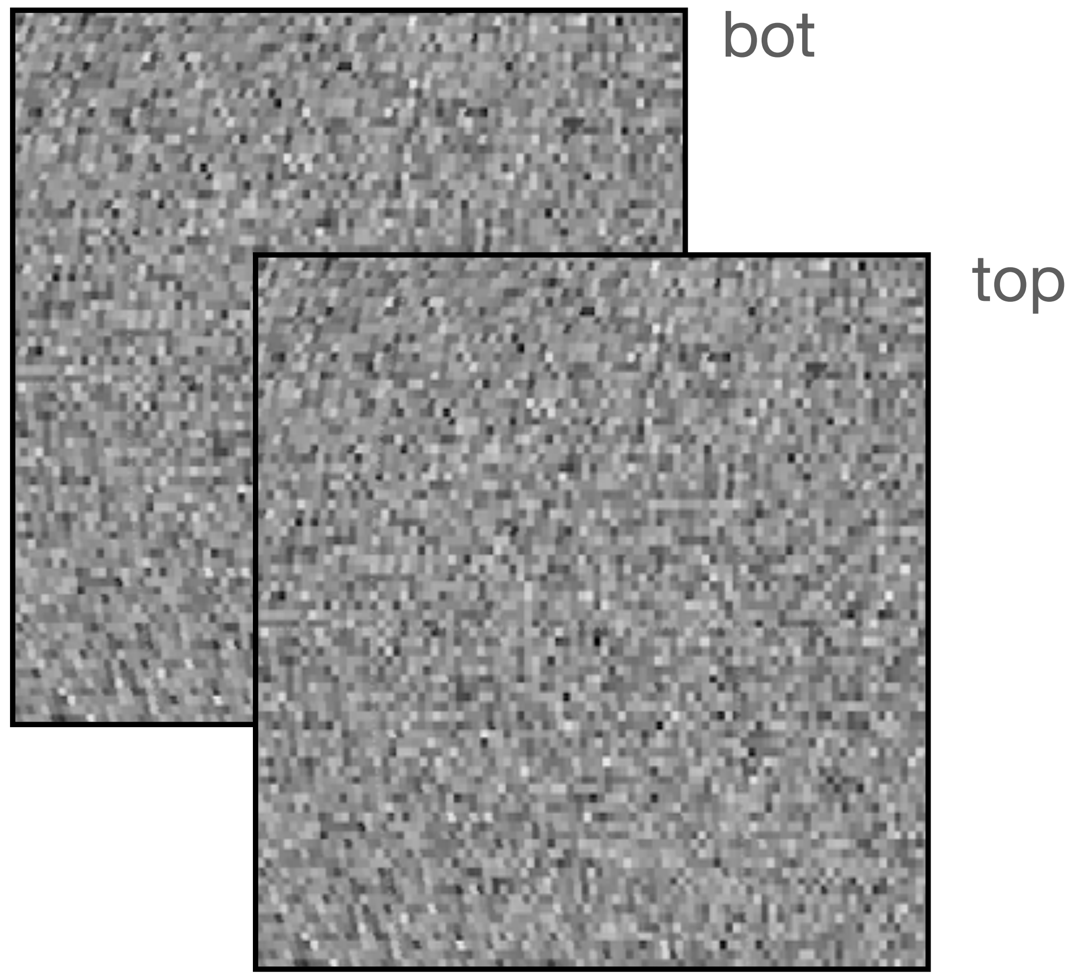
$$\Sigma_i$$

Compute (local)
conditional covariance
matrix

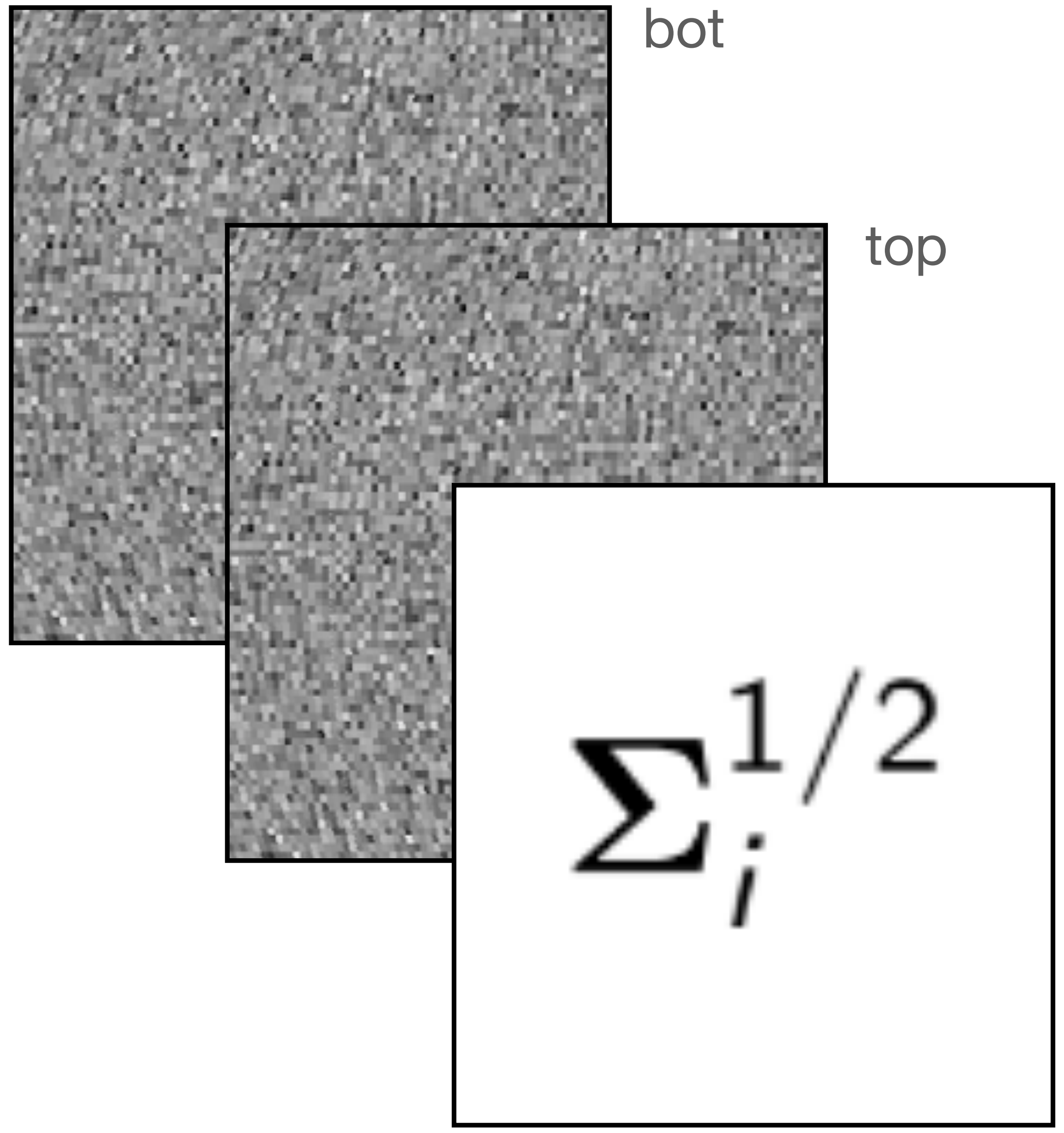
Obtaining uncertainties is facilitated by local conditional simulations



Simulate Gaussian white noise over grid (keep fixed)

$$\Sigma_i$$

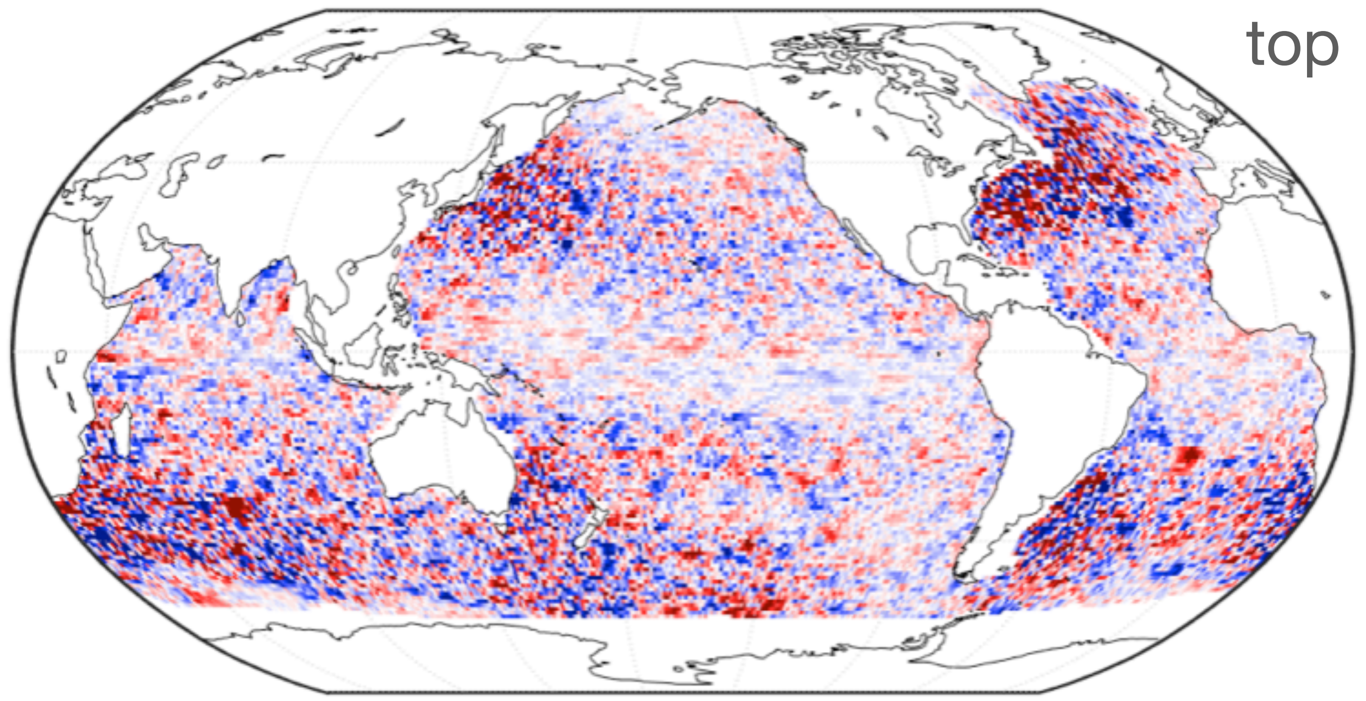
Compute (local) conditional covariance matrix

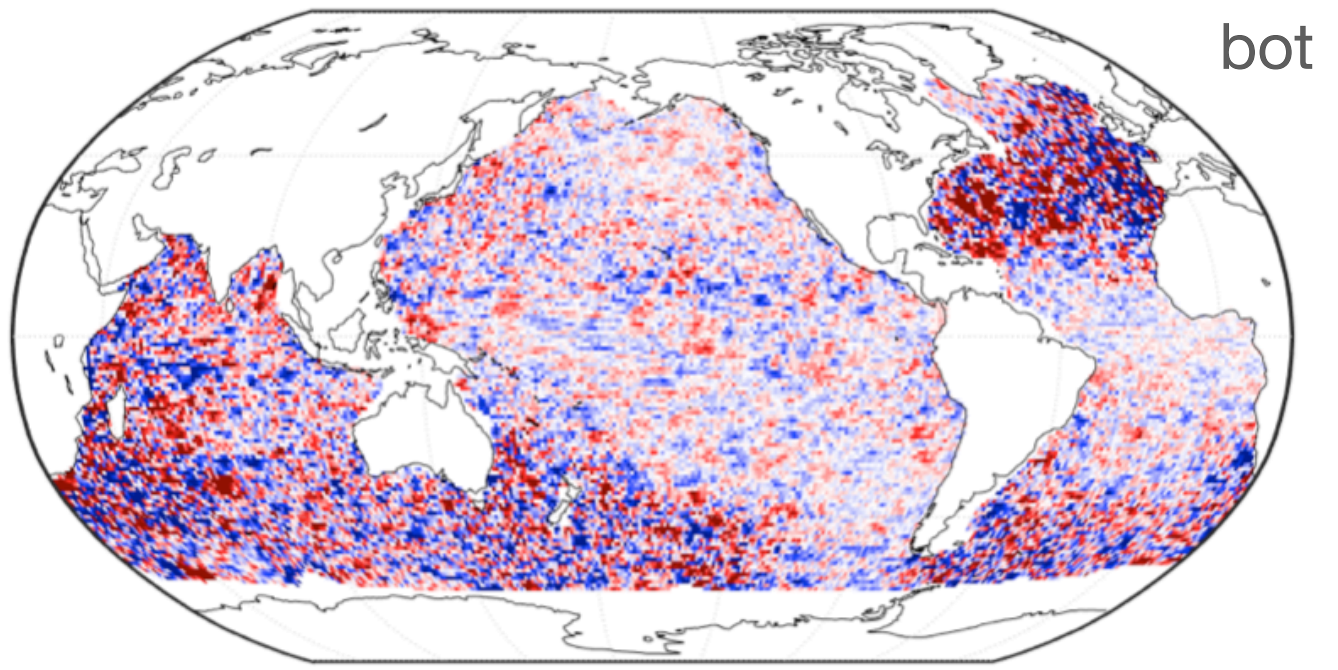


$$\Sigma_i^{1/2}$$

Take symmetric square root and multiply by white noise

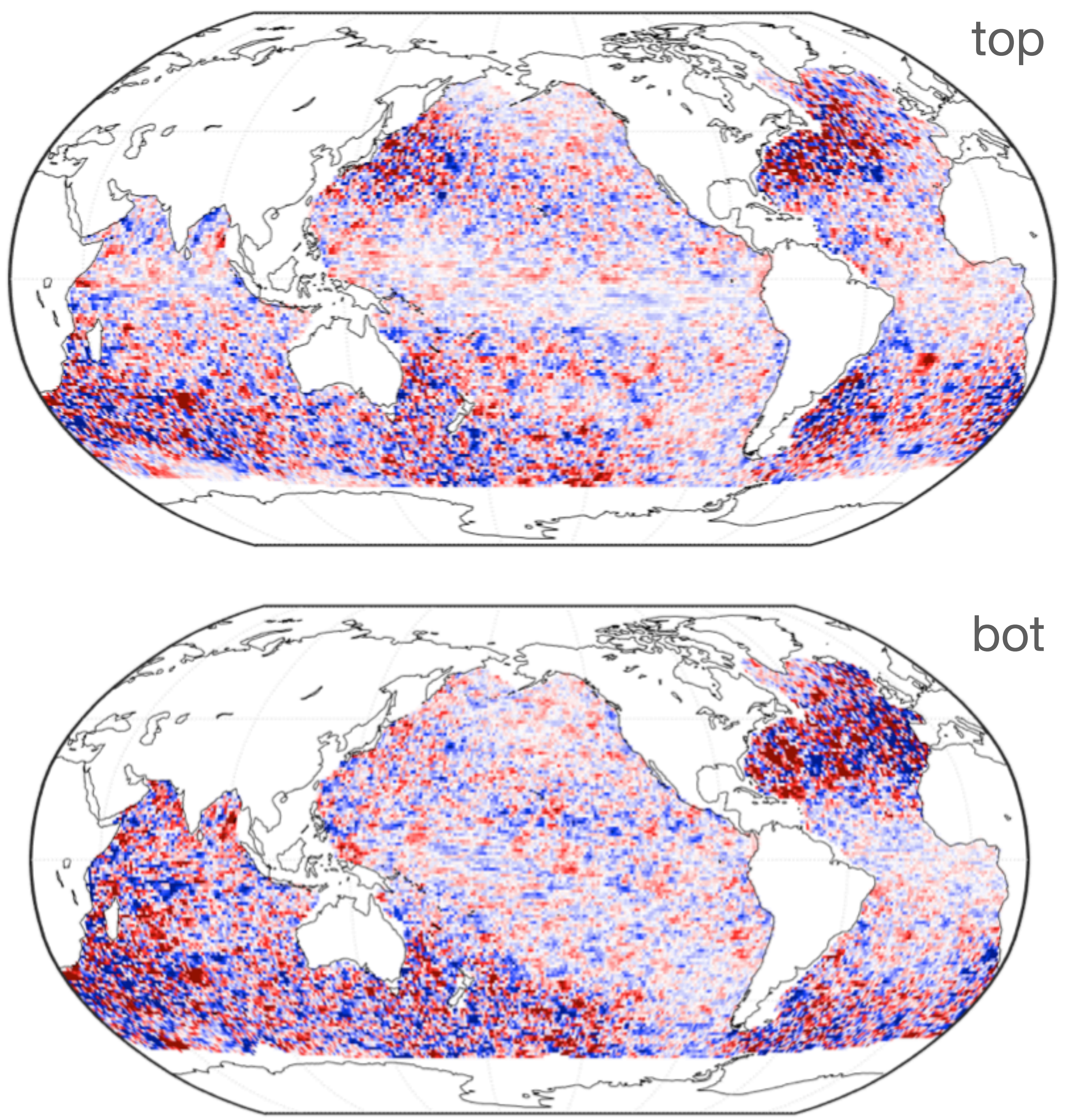
Obtaining uncertainties is facilitated by local conditional simulations





Keep the center point and repeat for all grid points

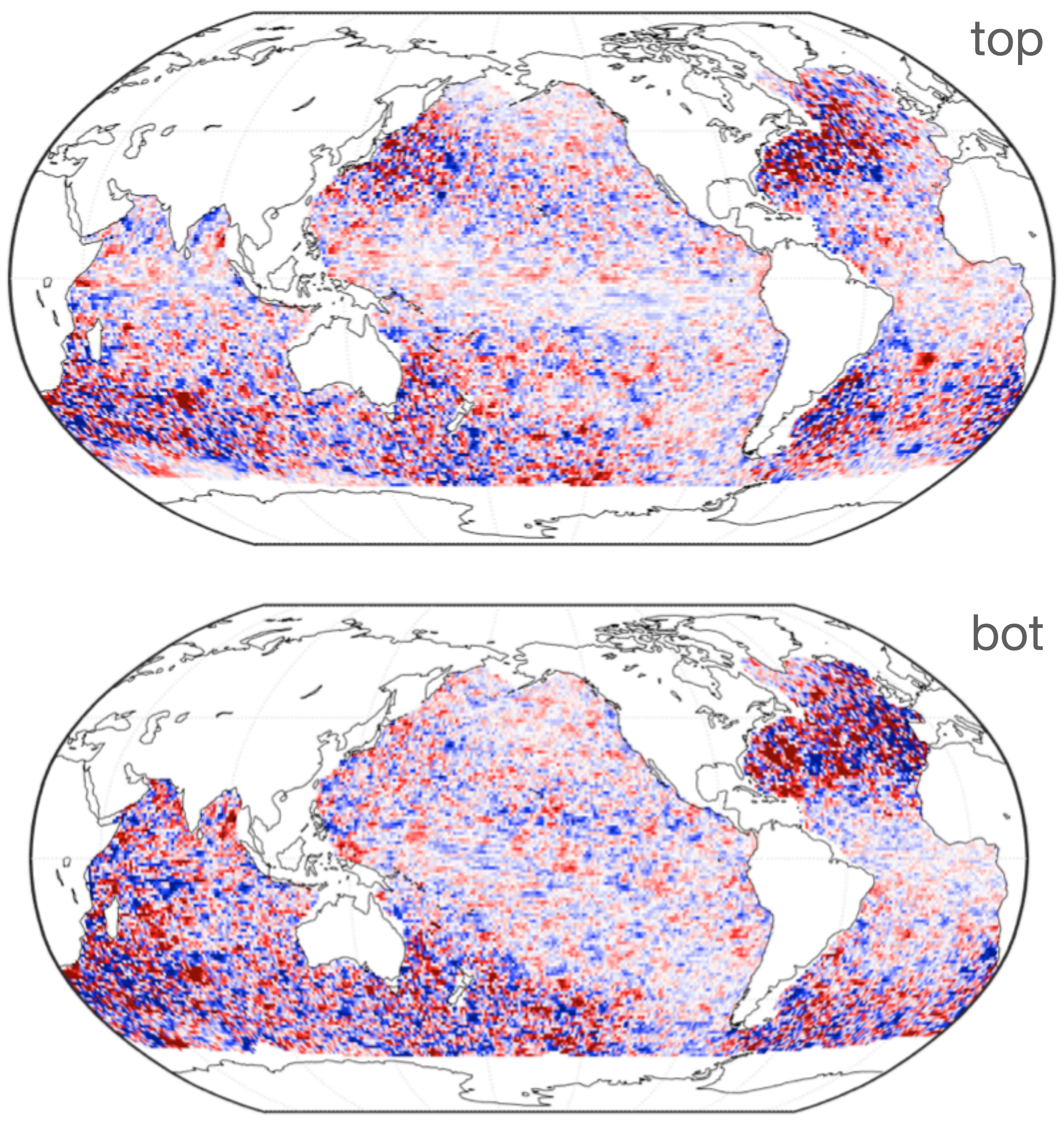
Obtaining uncertainties is facilitated by local conditional simulations



Keep the center point and repeat for all grid points

Repeat for desired number of ensemble members

Obtaining uncertainties is facilitated by local conditional simulations



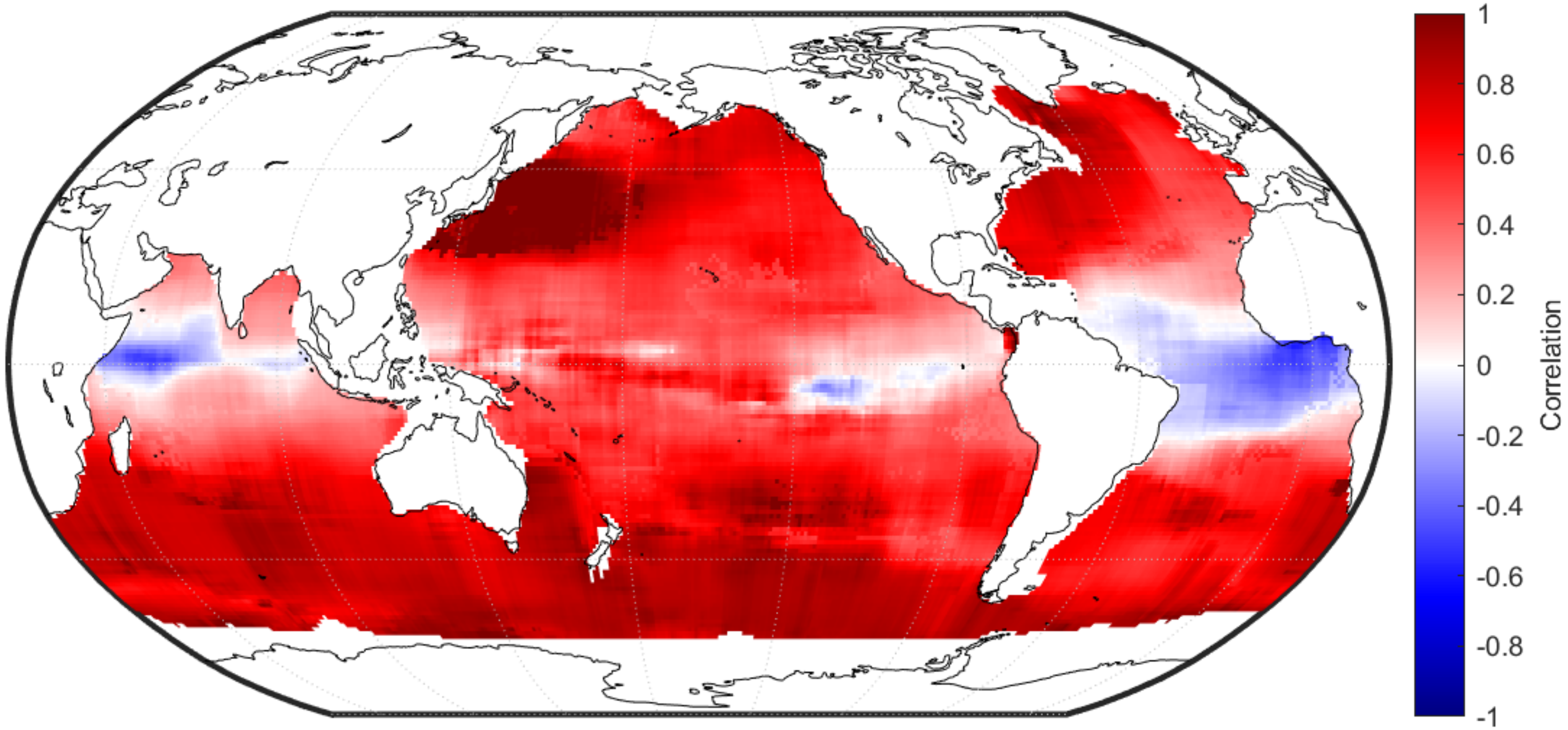
Keep the center point and repeat for all grid points

Repeat for desired number of ensemble members

We modeled the correlation, so sample variance of top + bottom layer integrated ensemble members is estimate of

$$\mathrm{Var}(\mathrm{OHC}_{\mathrm{total}}|\mathrm{data})$$

Most ocean regions' temperatures are positively correlated



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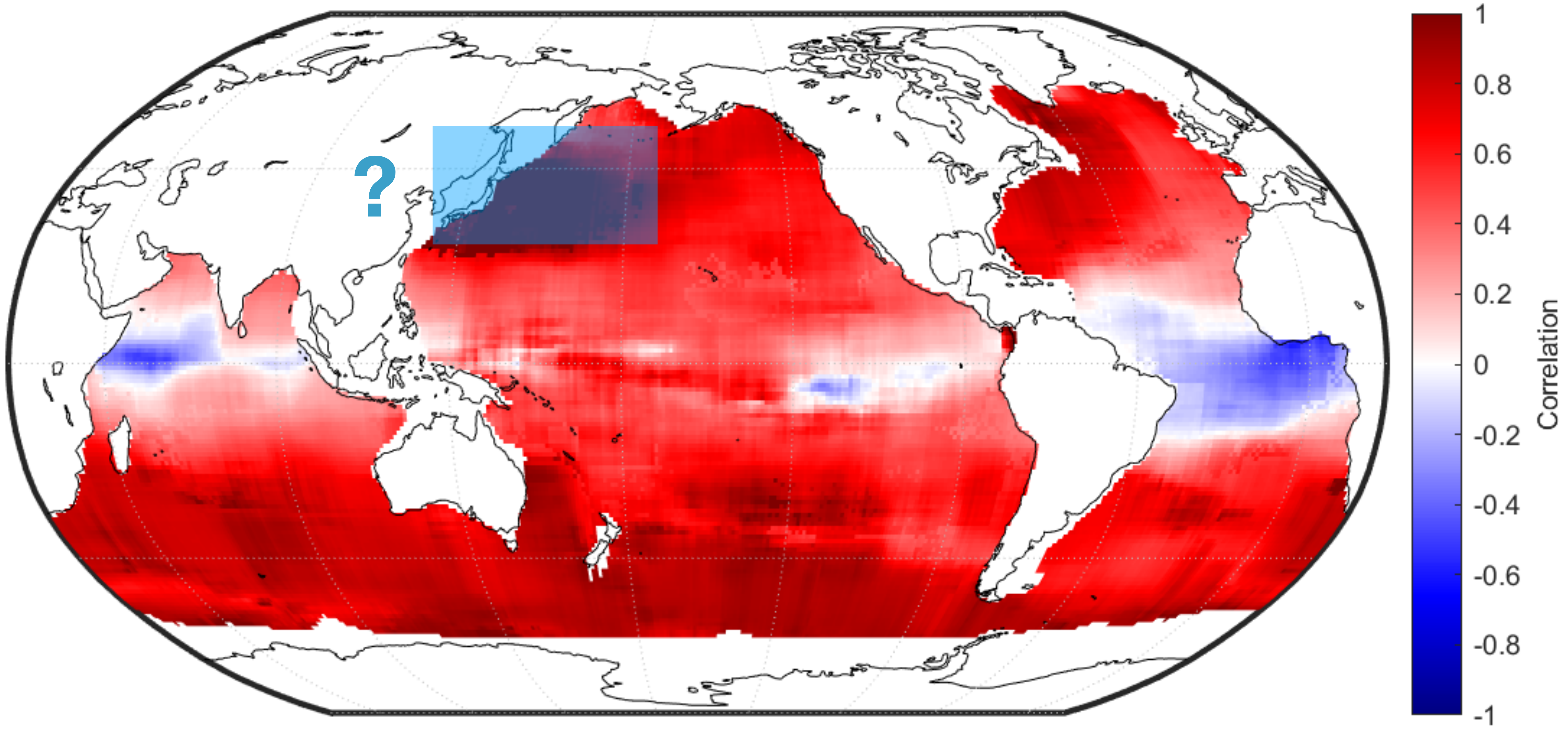
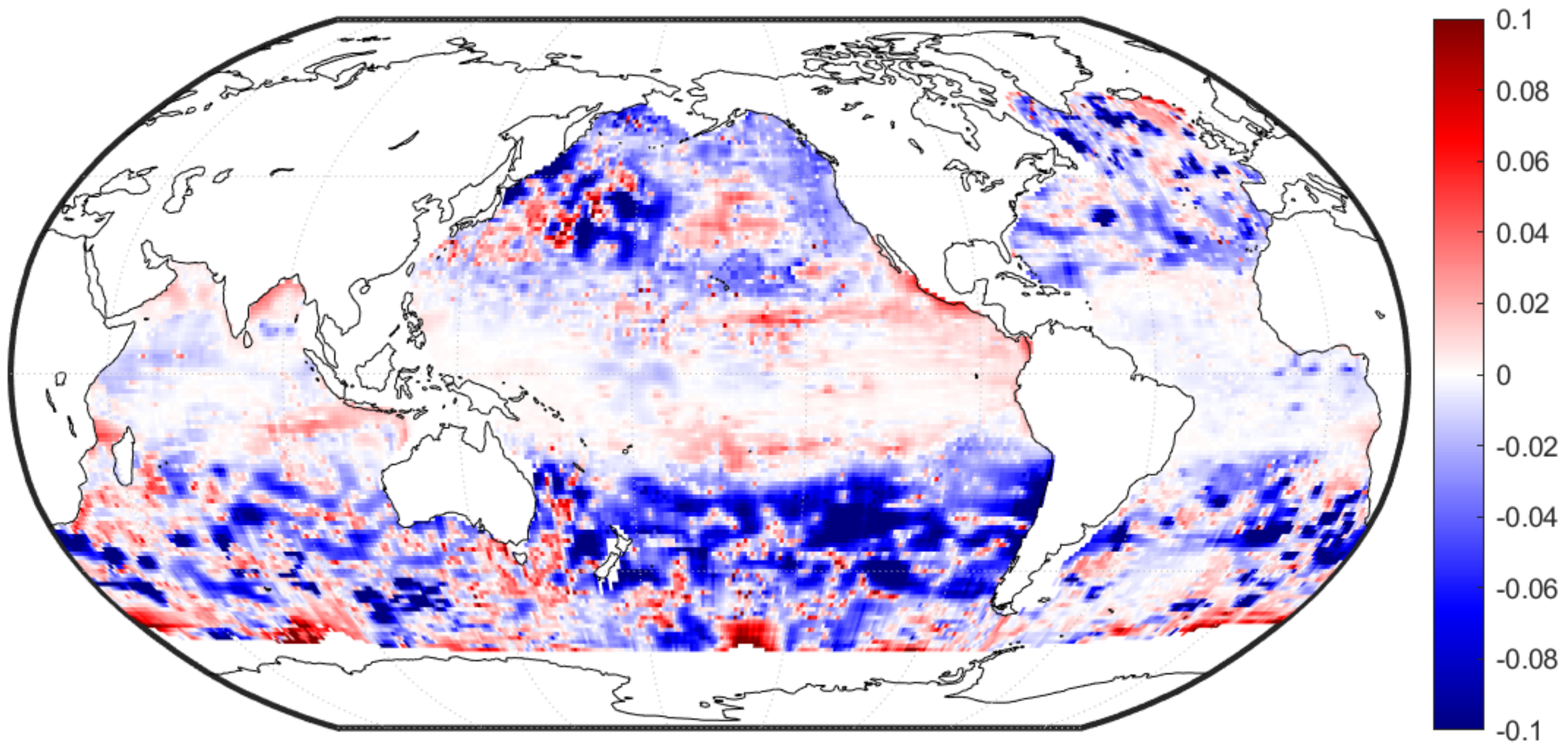
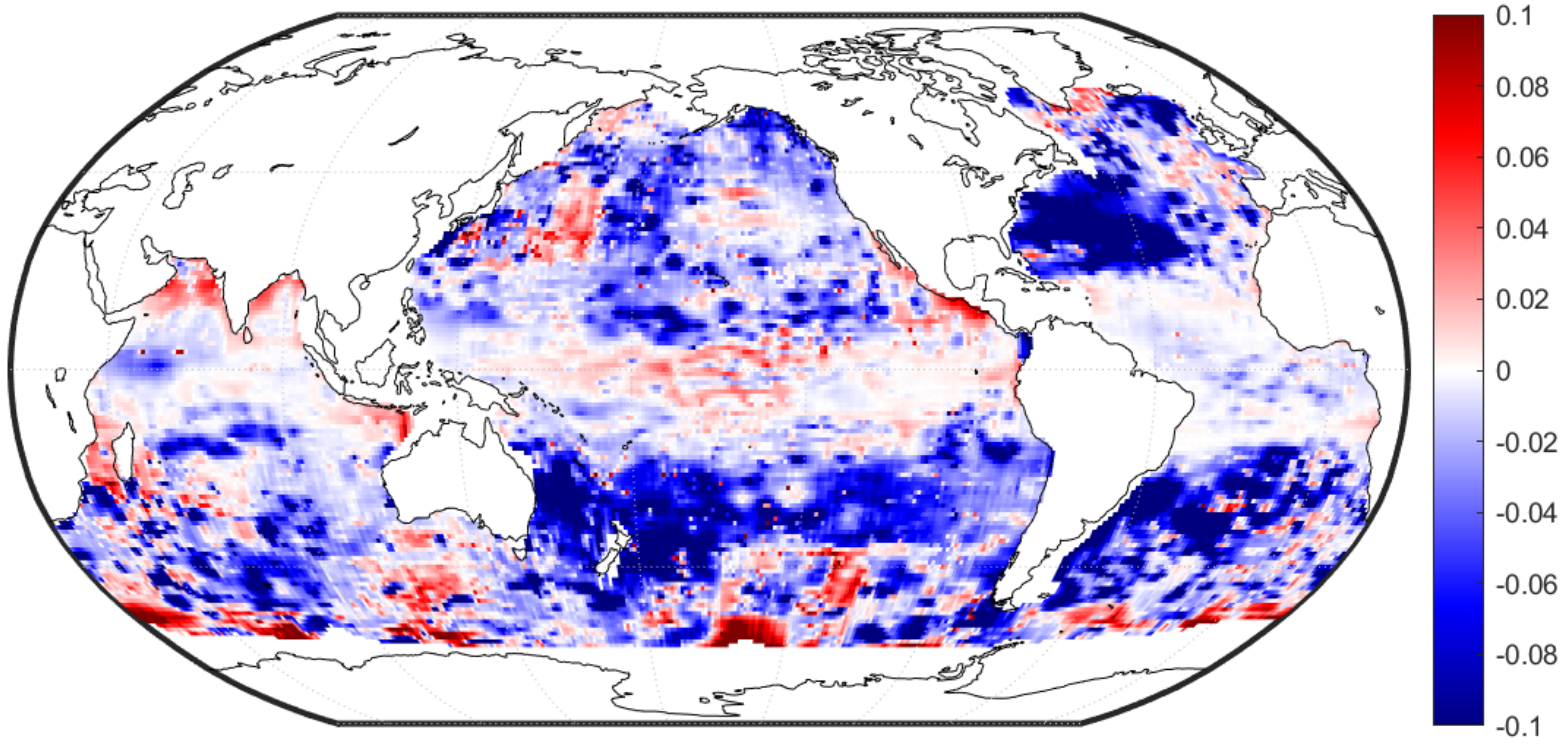


The bivariate model tends to produce lower kriging variances

$$\frac{\text{bivariate kriging variance - univariate kriging variance}}{\text{univariate kriging variance}} \quad (02/2010)$$



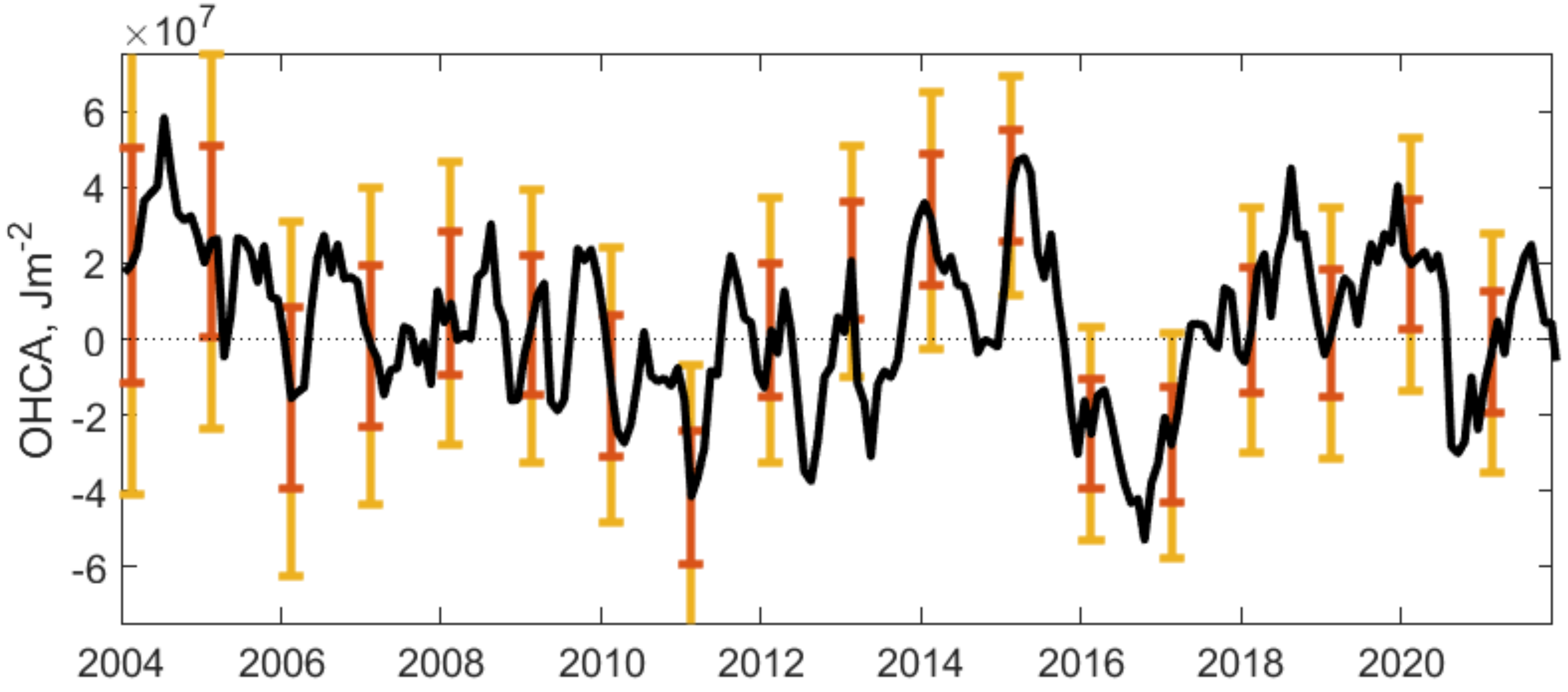
Top layer



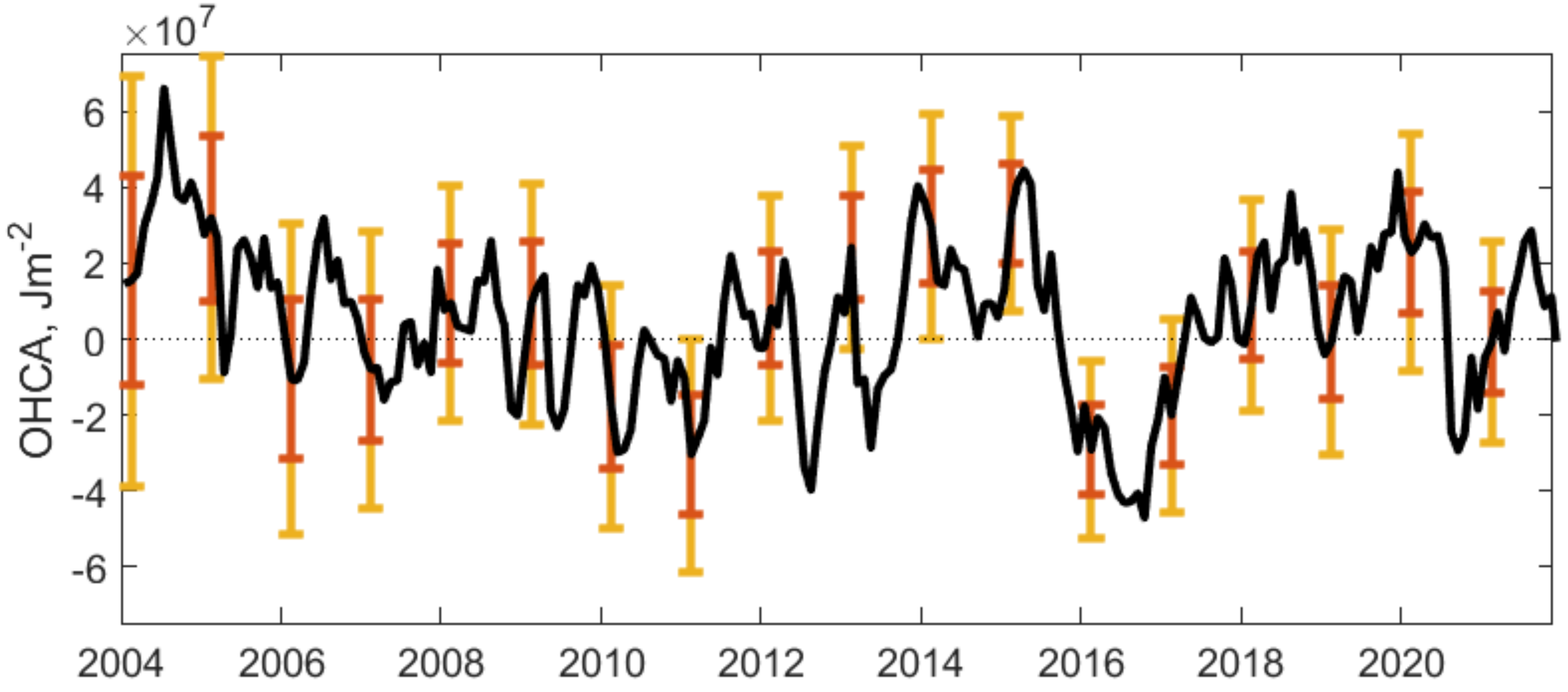
Bottom layer

Bivariate total (top + bottom) OHC uncertainties tend to be ~15% smaller than univariate

Global OHC anomaly estimates

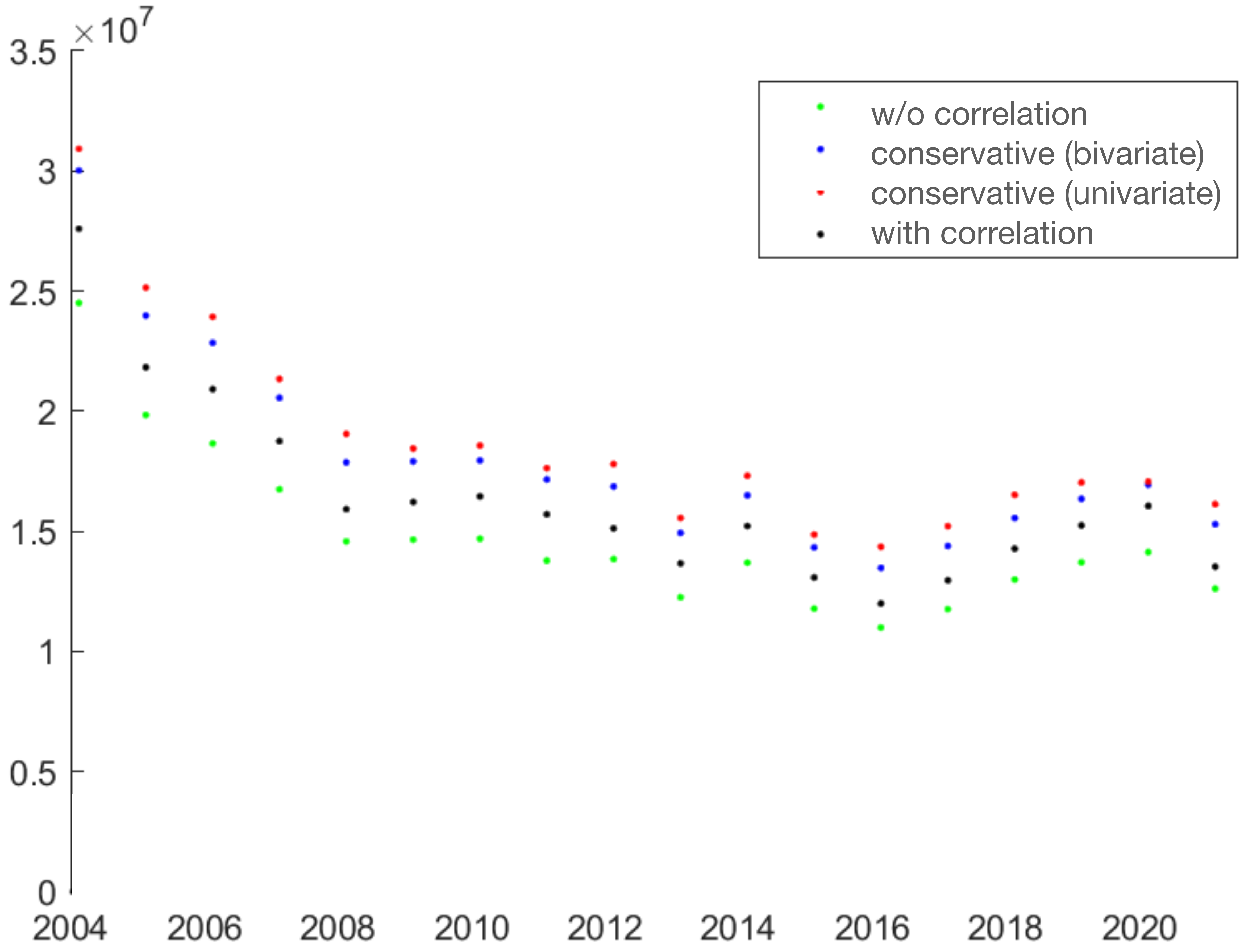


Univariate



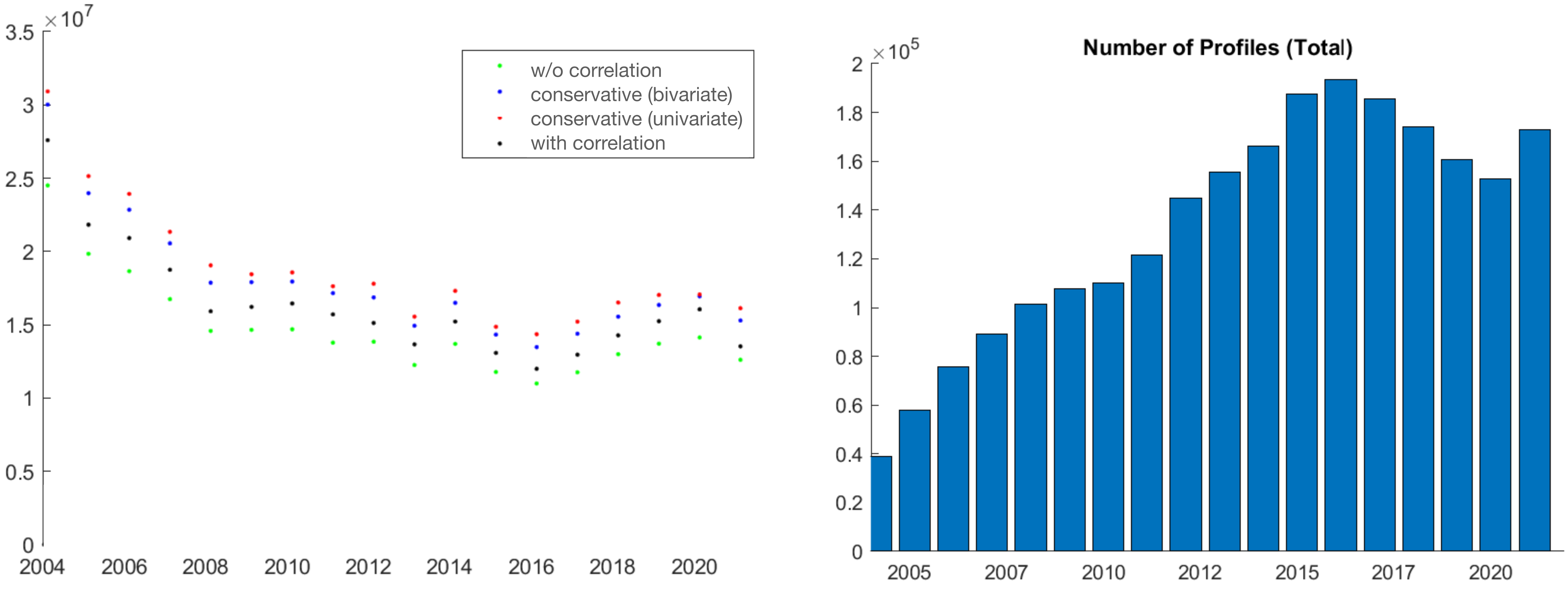
Bivariate

Bivariate total (top + bottom) OHC uncertainties tend to be ~15% smaller than univariate

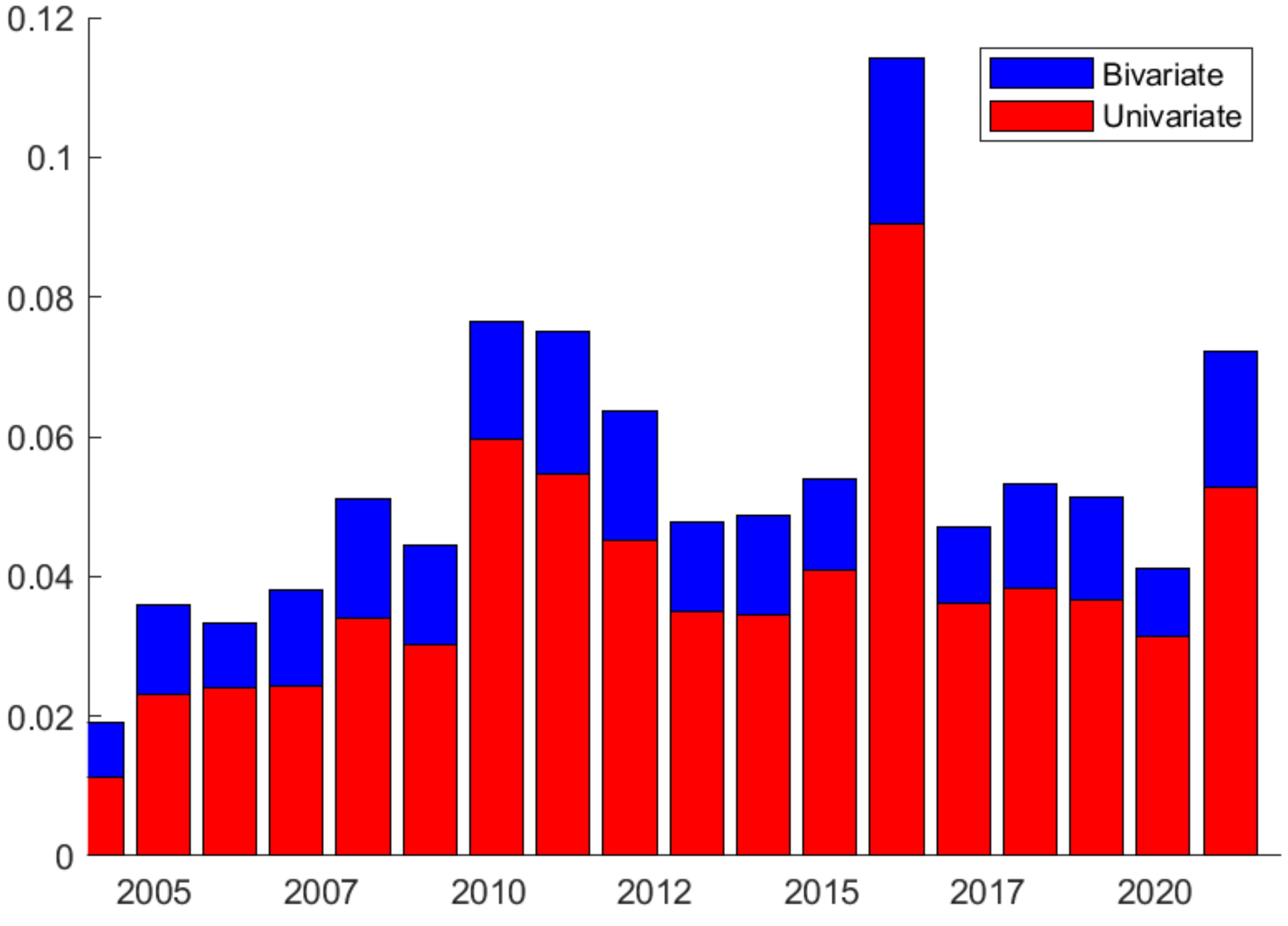


When we model the correlation, the uncertainties are **smaller** than the conservative and **larger** than those w/o the correlation.

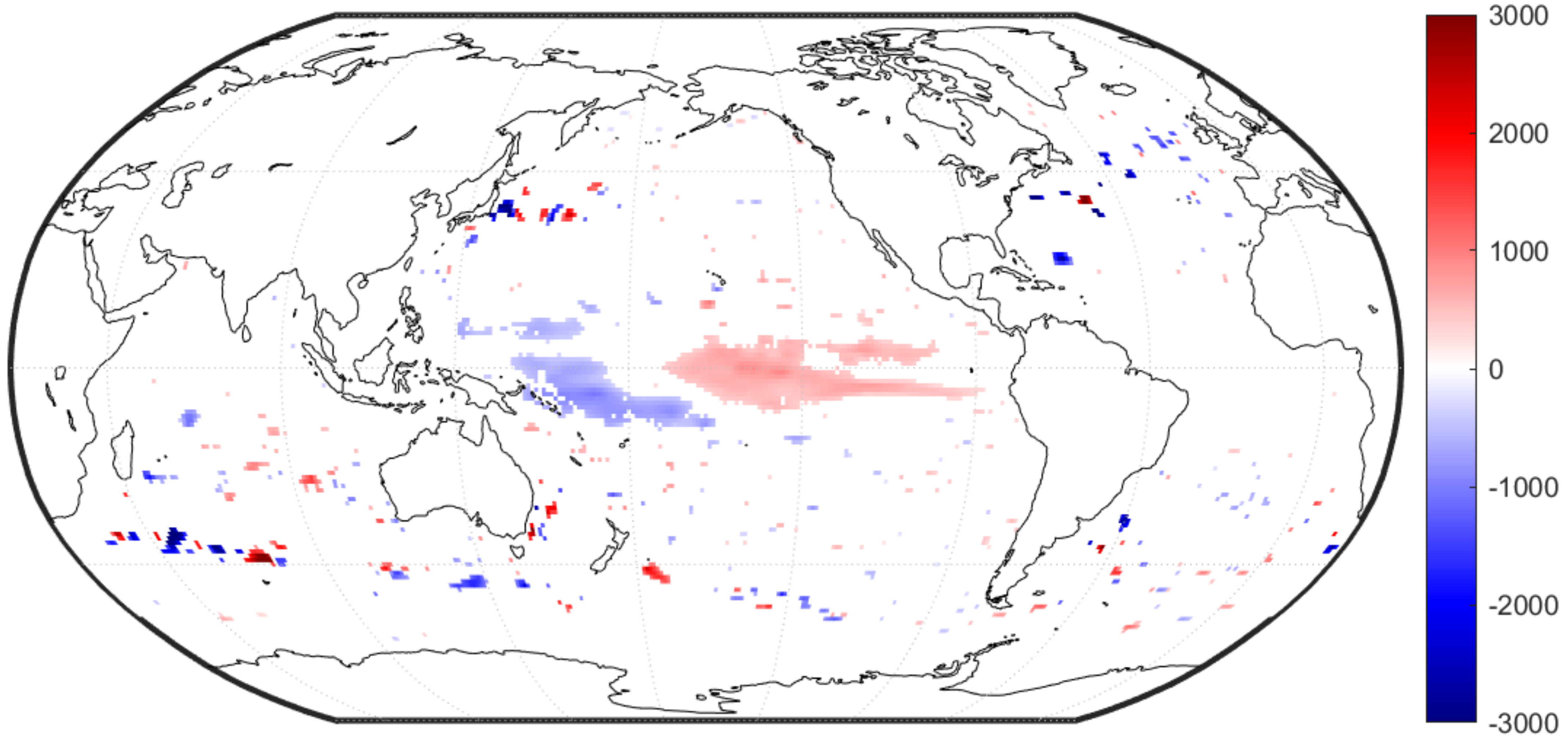
The uncertainty trend follows the number of profiles/floats



The equatorial OHC anomalies are consistently significant

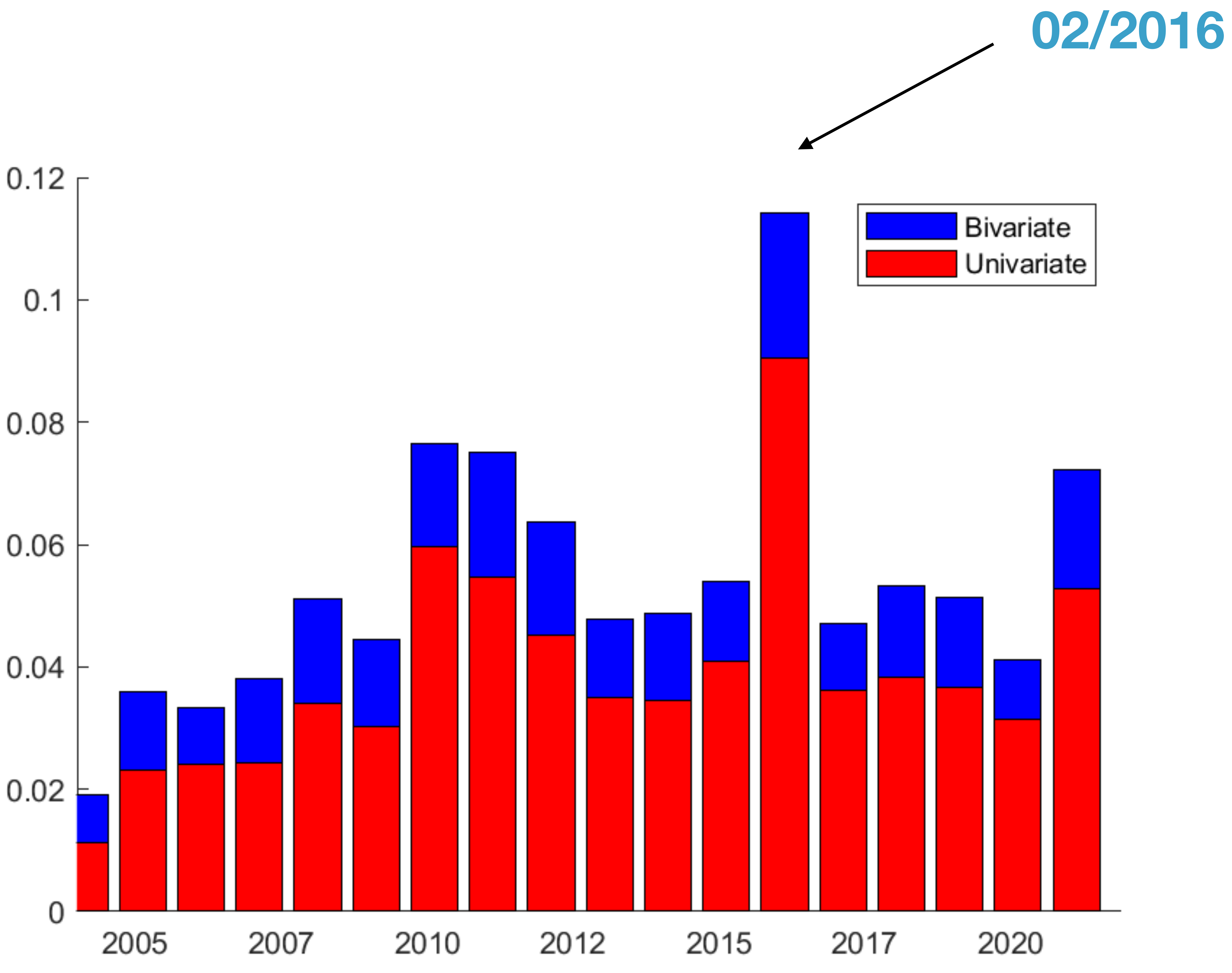


Proportion of significant grid points over time (95% level)



Significant temperature anomalies (02/2010)

The equatorial OHC anomalies are consistently significant



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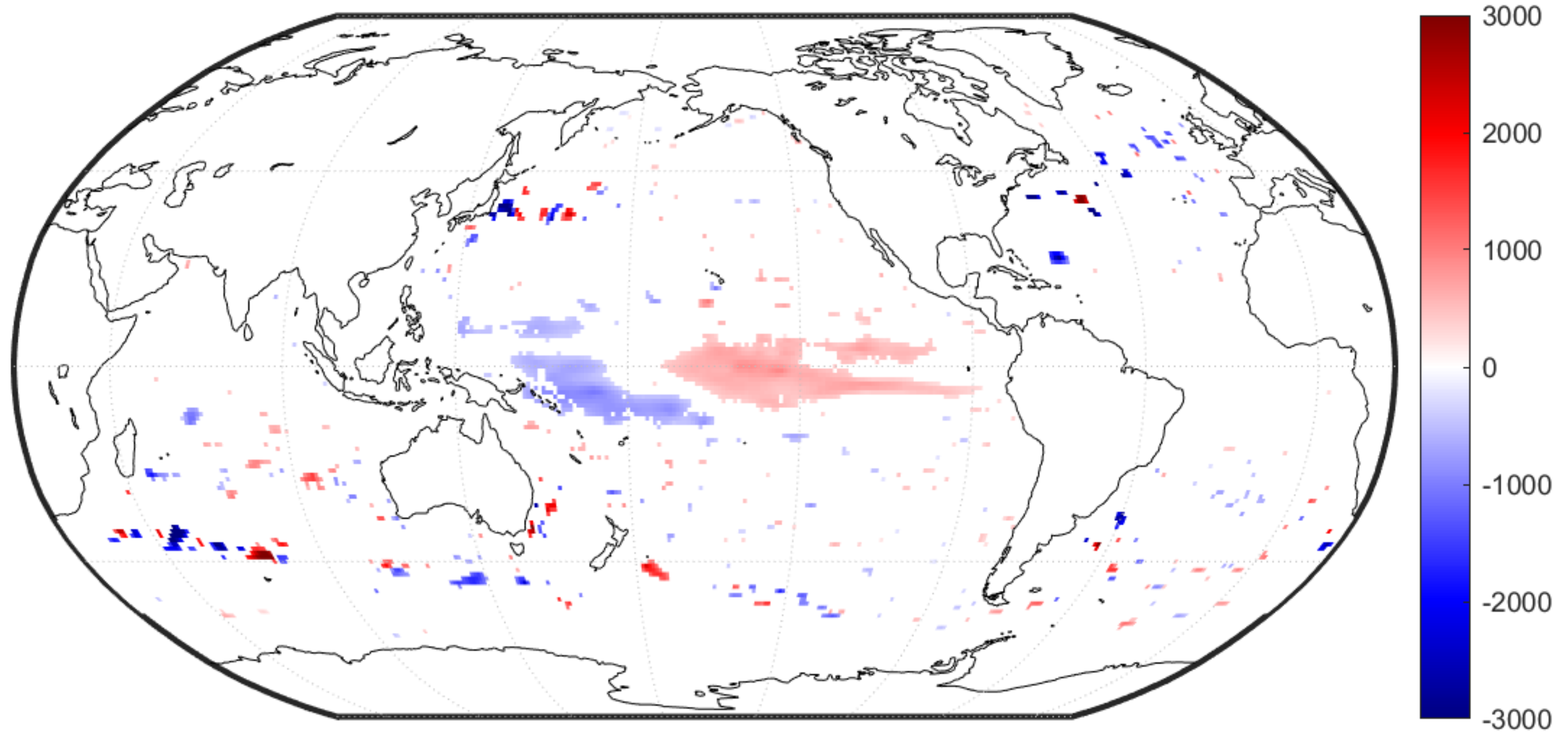
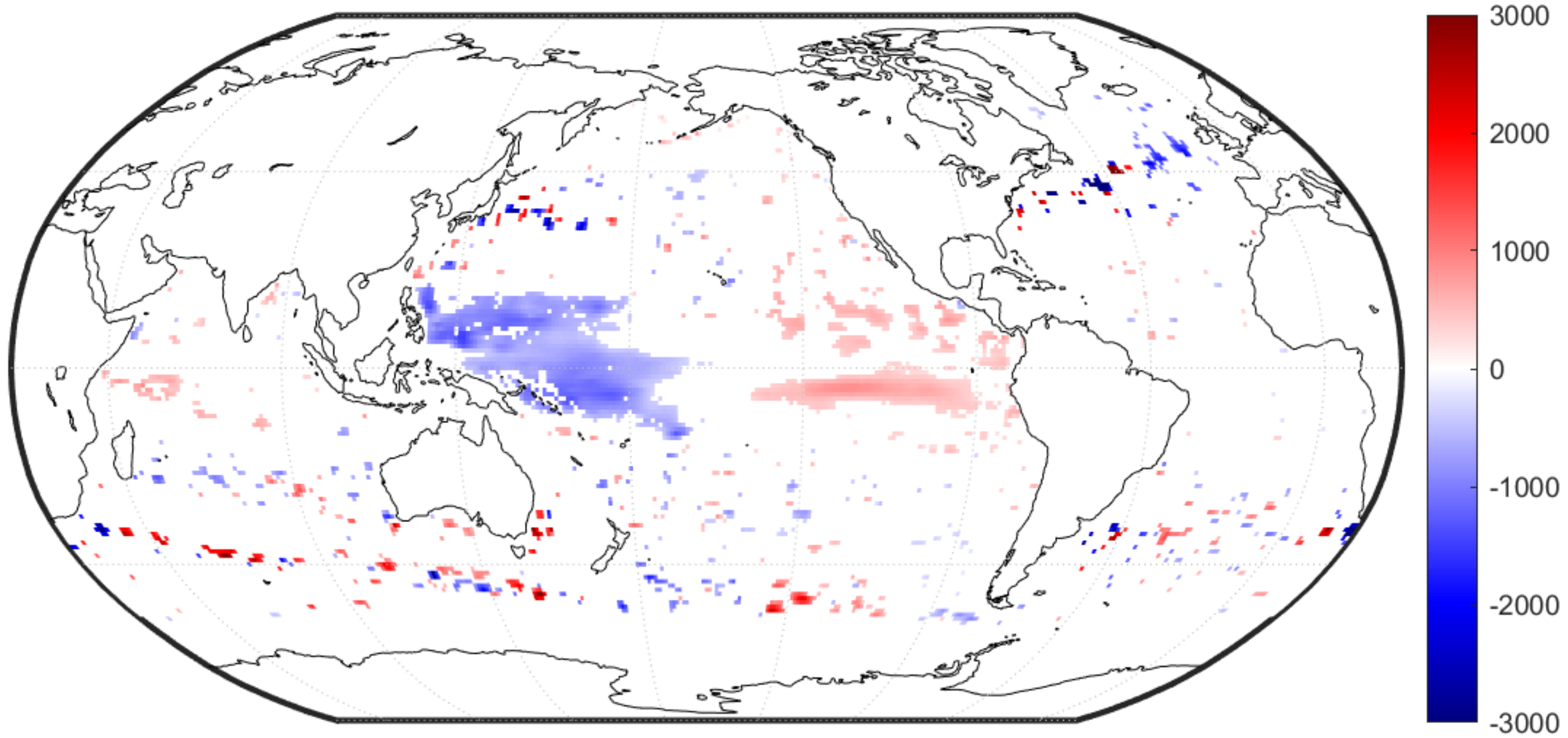
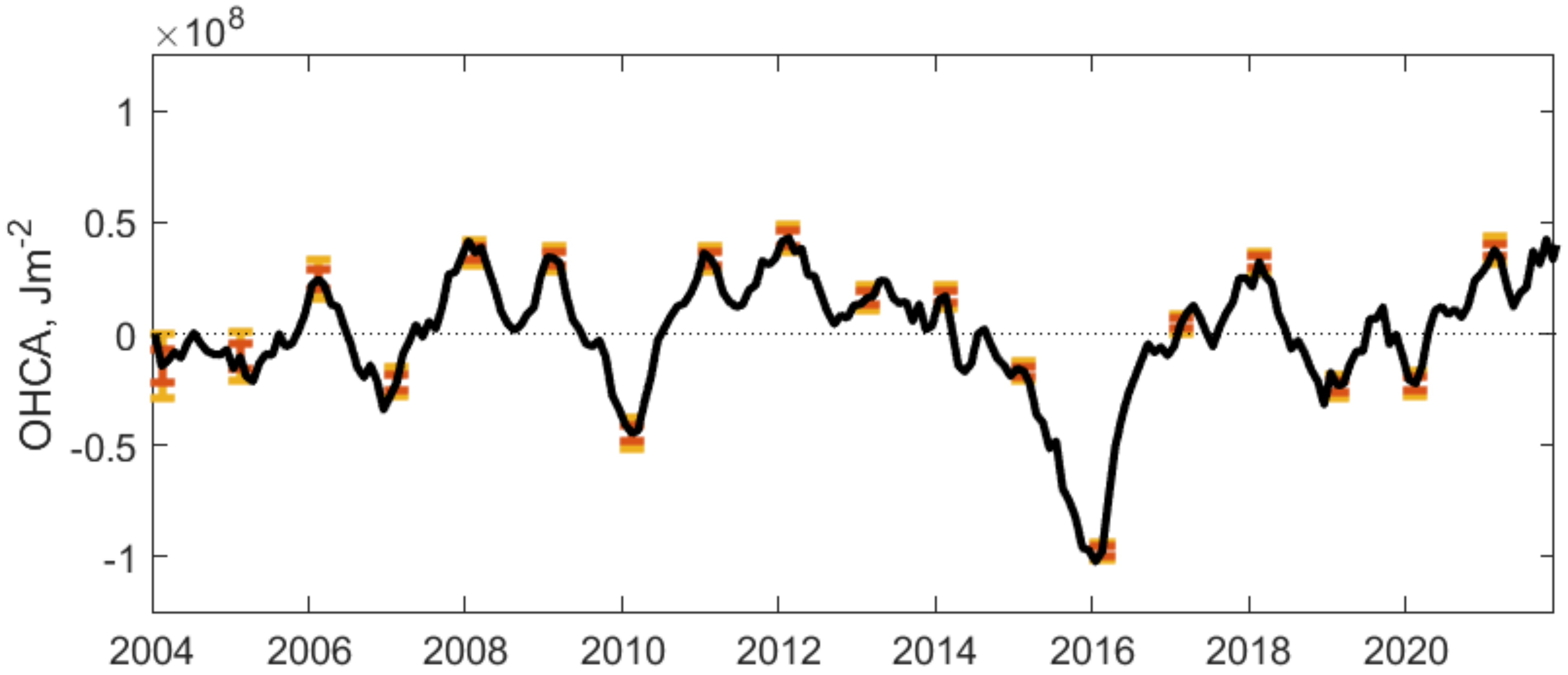


Significant temperature anomalies (02/2010)

The 2015-16 El Niño appears in the equatorial OHC anomalies

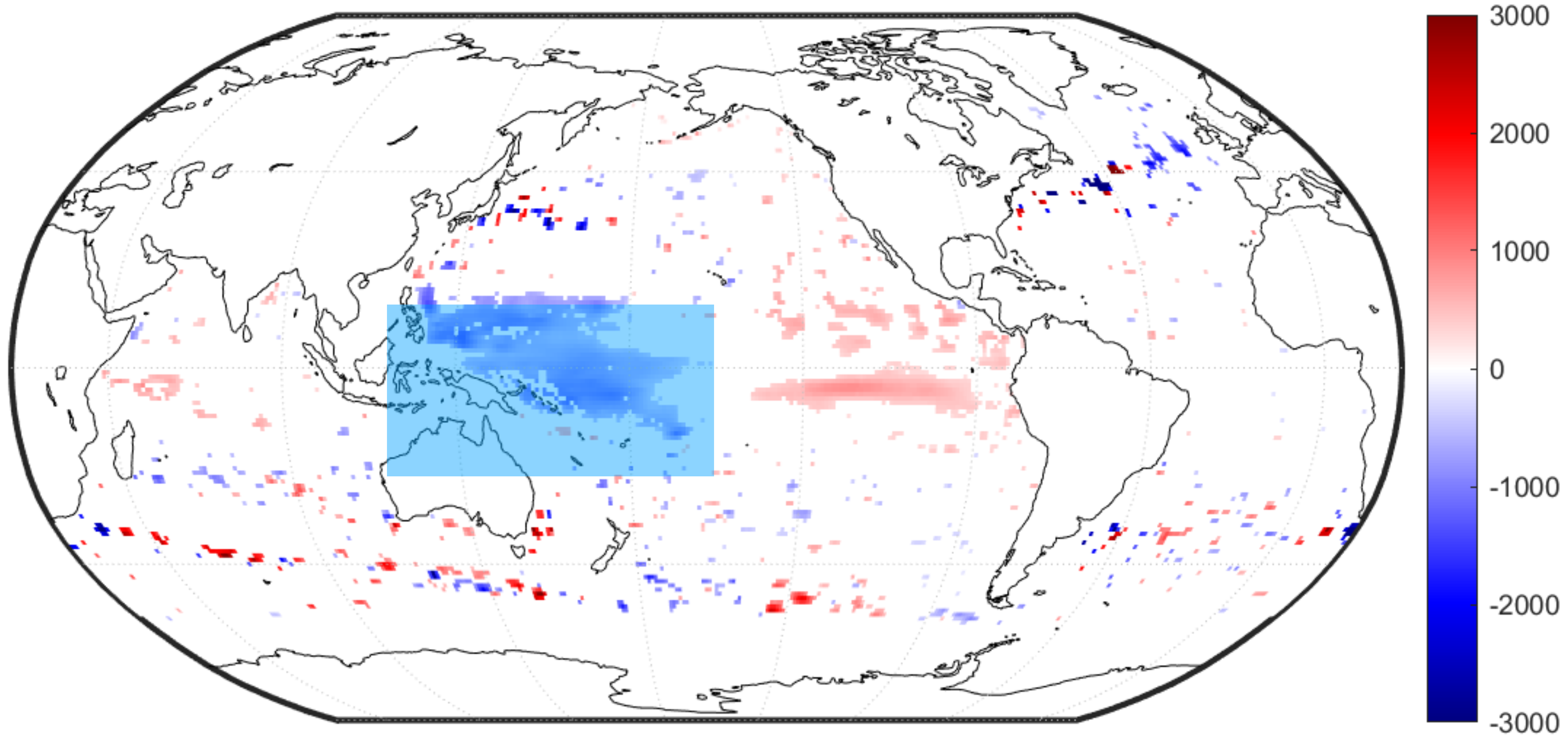


Significant temperature anomalies (02/2016)

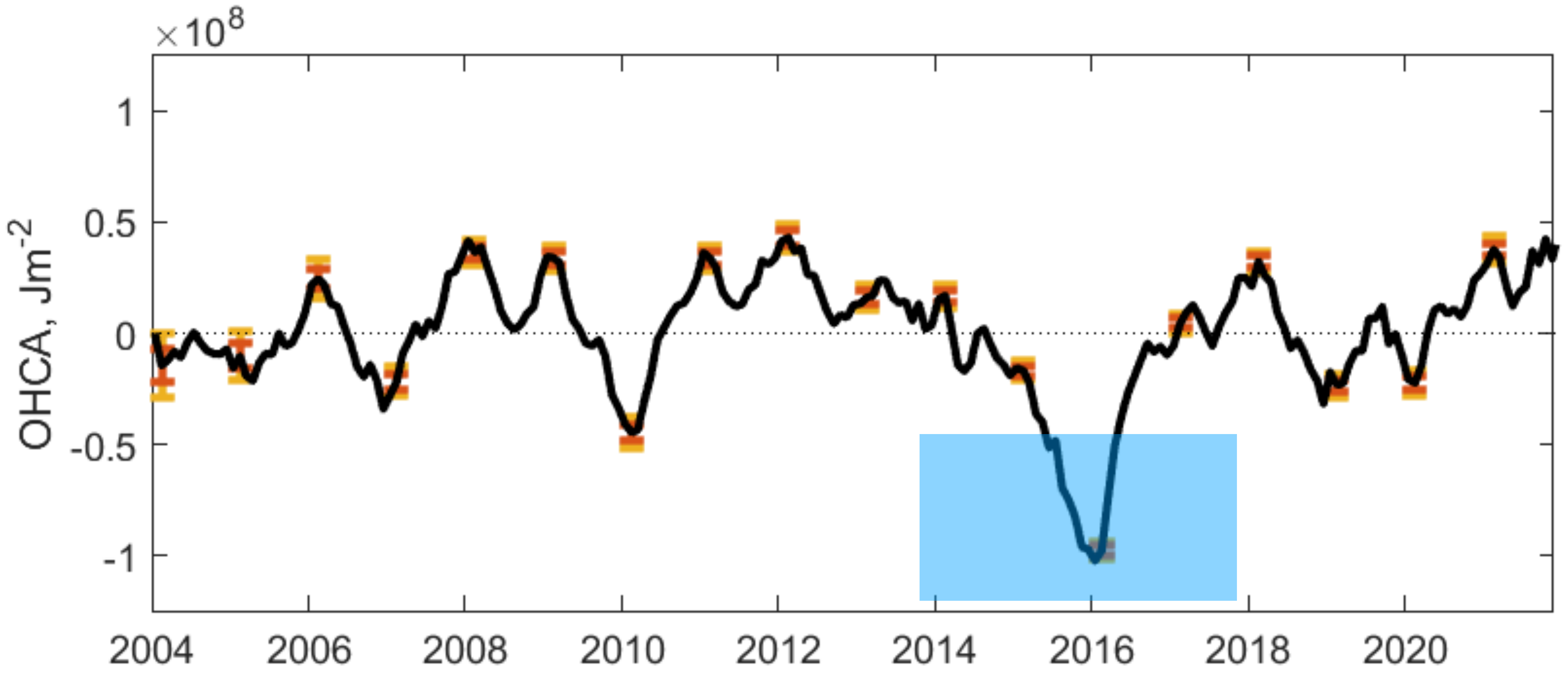


Western Equatorial Pacific OHC anomalies

The 2015-16 El Niño appears in the equatorial OHC anomalies



Significant temperature anomalies (02/2016)



Western Equatorial Pacific OHC anomalies

Future work

- Validate kriging variances and uncertainties
    - Cross-validation
    - Mapping synthetic profiles and comparing to model truth
- Investigate the Kuroshio region (account for non-Gaussianity?)
- Uncertainties for mean field and climatological time trend
- Generalize GP regression model to more than two layers
- Apply model to other fields (e.g. SSH and OHC, oxygen and T/S)

Summary

- Estimating ocean heat content (with reliable uncertainties) is crucial for **tracking climate change**

- Due to having fewer observations deeper in the water column, we model the OHC in the top and bottom layers **separately**

- To model the uncertainties of the total OHC in the water column (top + bottom) we need to estimate the spatially-varying cross-layer **correlation**

- Empirically, using a bivariate GP model to estimate the correlation reduces the OHC anomaly uncertainties both for each layer separately and ~15% in the water column (top + bottom)

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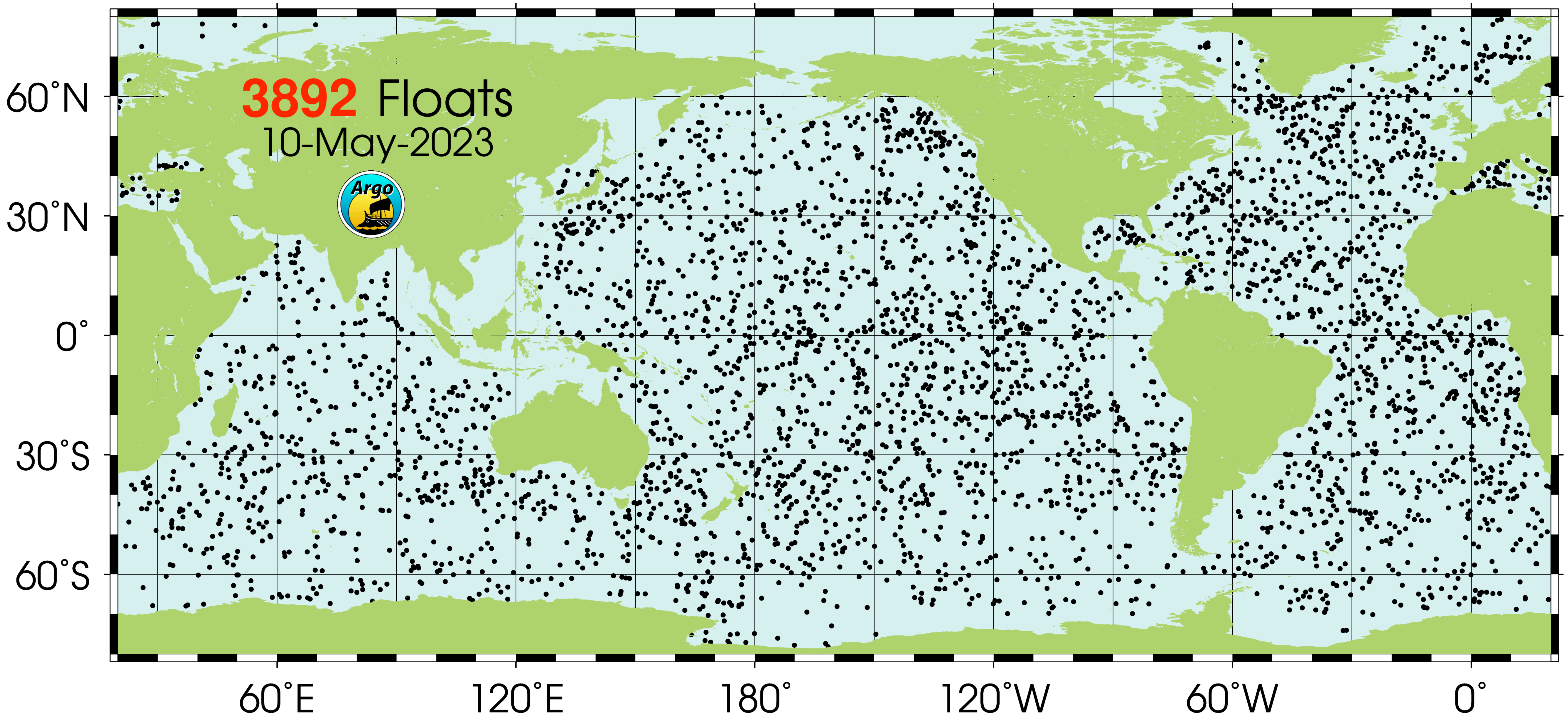
Thank you!

Backup

Argo floats are the state-of-the-art in ocean temperature measurements



(Argo Program)

The implementation is still computationally challenging

- For every grid point, use data in a 10 degree/3 month window
- Estimate GP model parameters numerically with MLE + BFGS algorithm
- How many grid points? **360 long x 180 lat = 64,800 grid points (!)**
- Embarrassingly parallel, but still computationally challenging
    - Fit parameters for 180 x 20 slice: **67h (desktop) / 8h (PSC)**
    - Obtain conditional simulations for Feb of every year: **~12h (desktop)**

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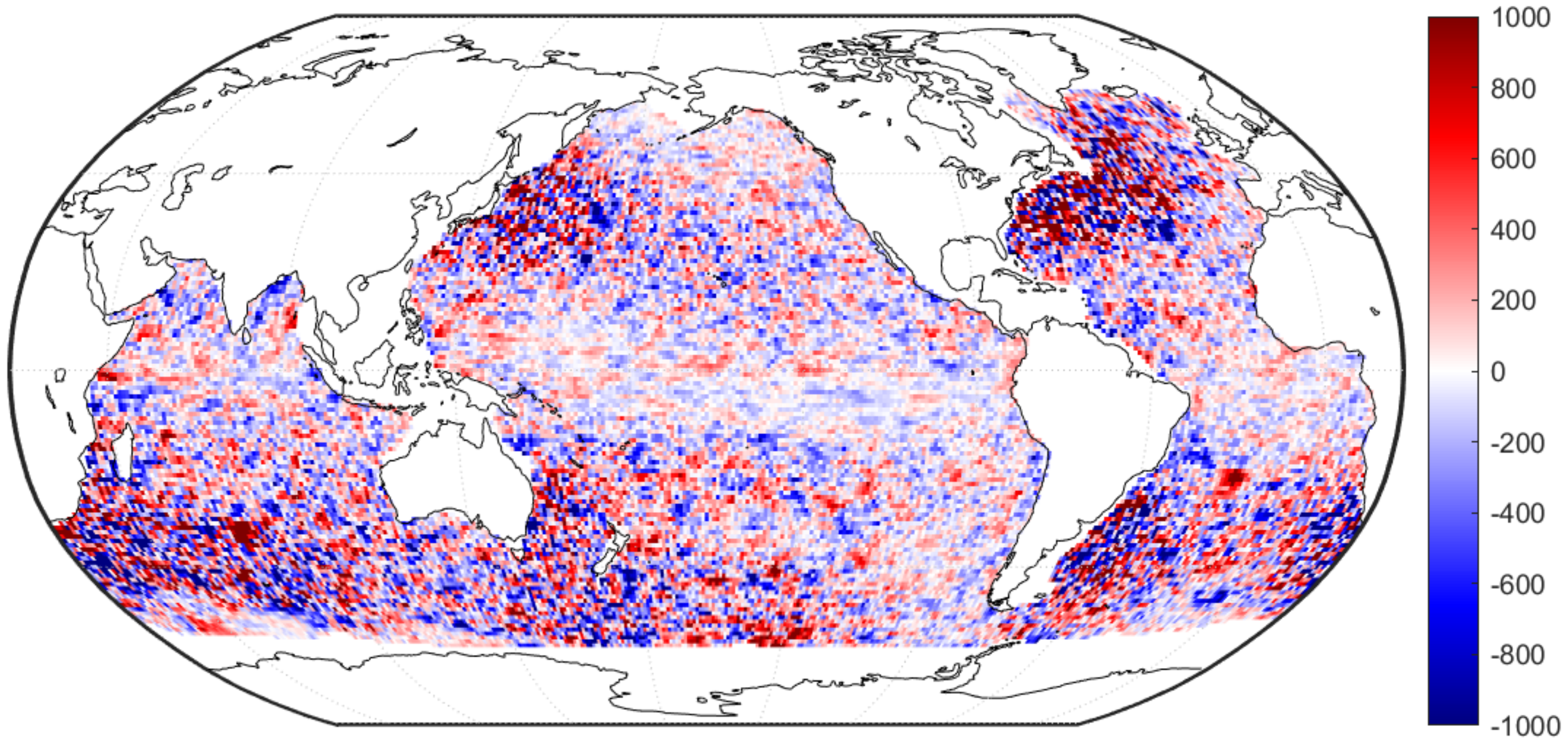
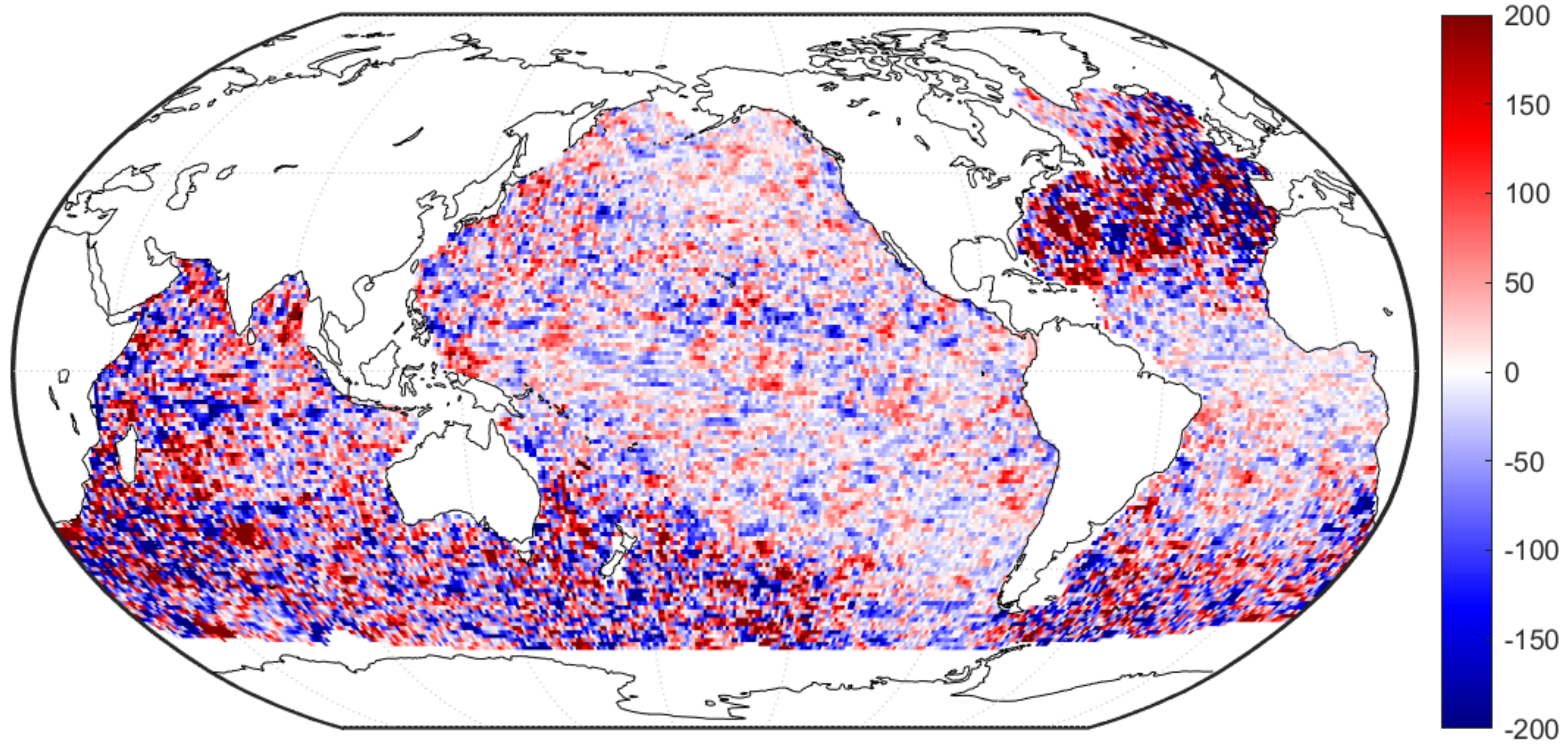
The bivariate uncertainties tend to be ~15% smaller than the univariate

Conditional simulation realization (02/2010)



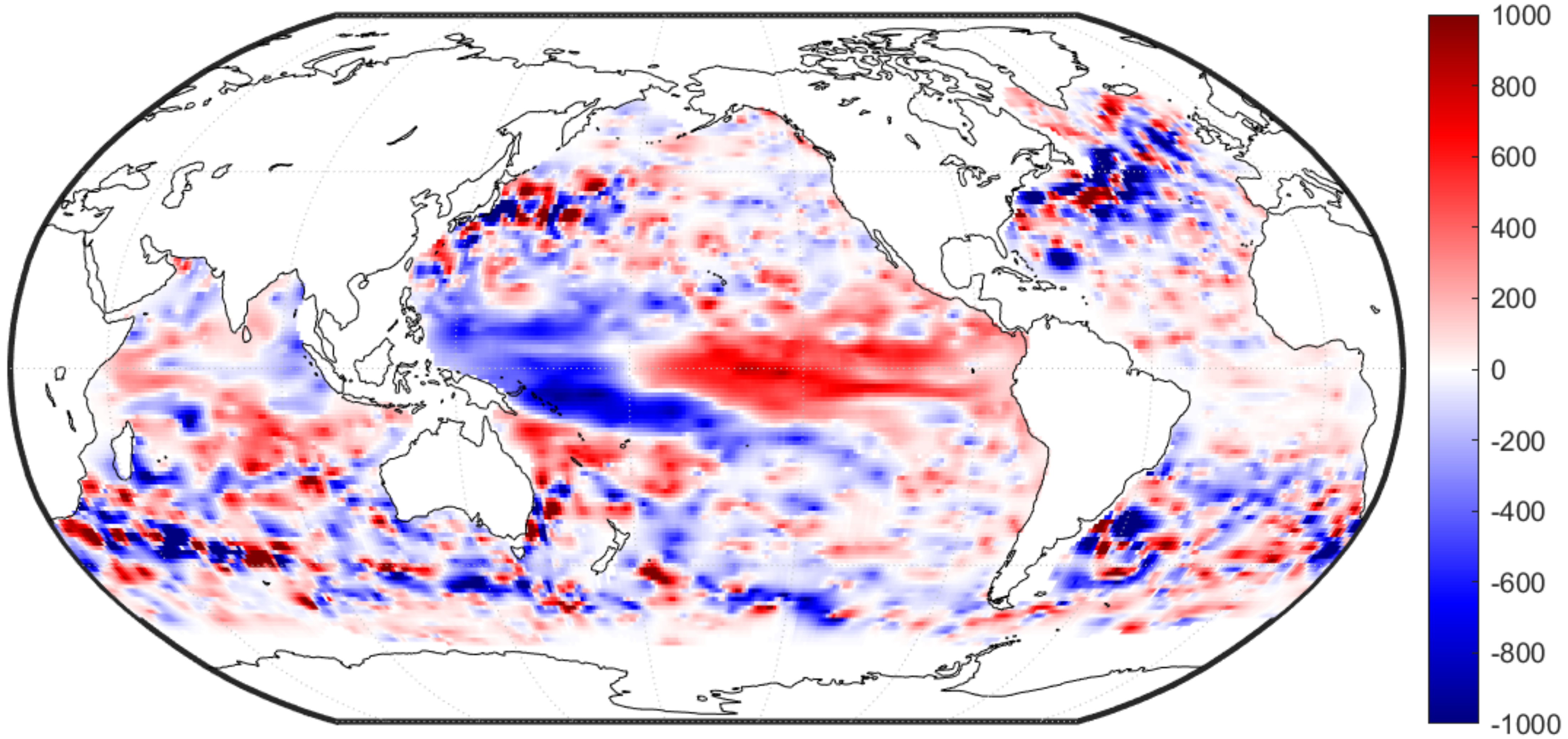
Upper ocean



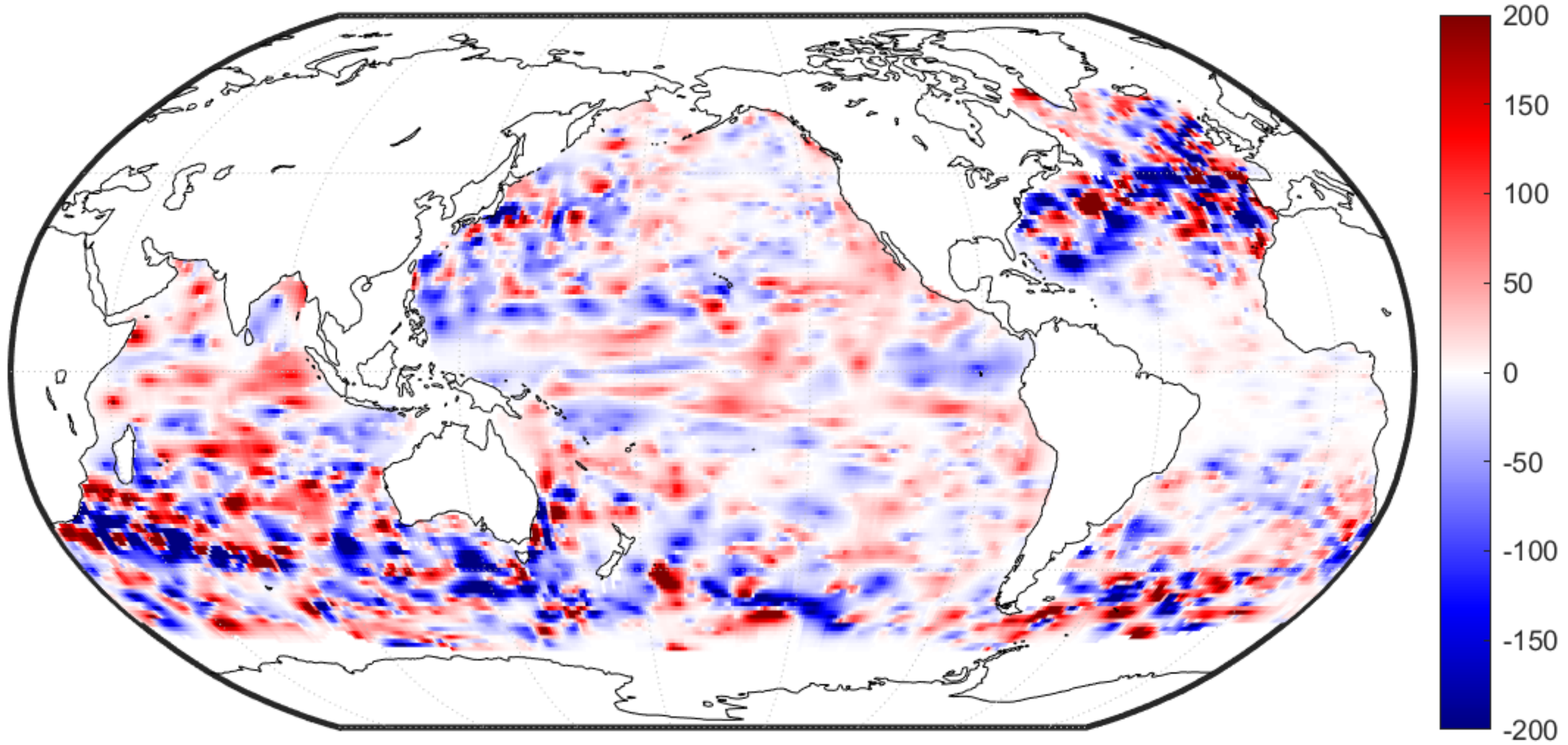
Mid-ocean

The bivariate model tends to produce lower kriging variances

Predicted temperature anomalies (02/2010)



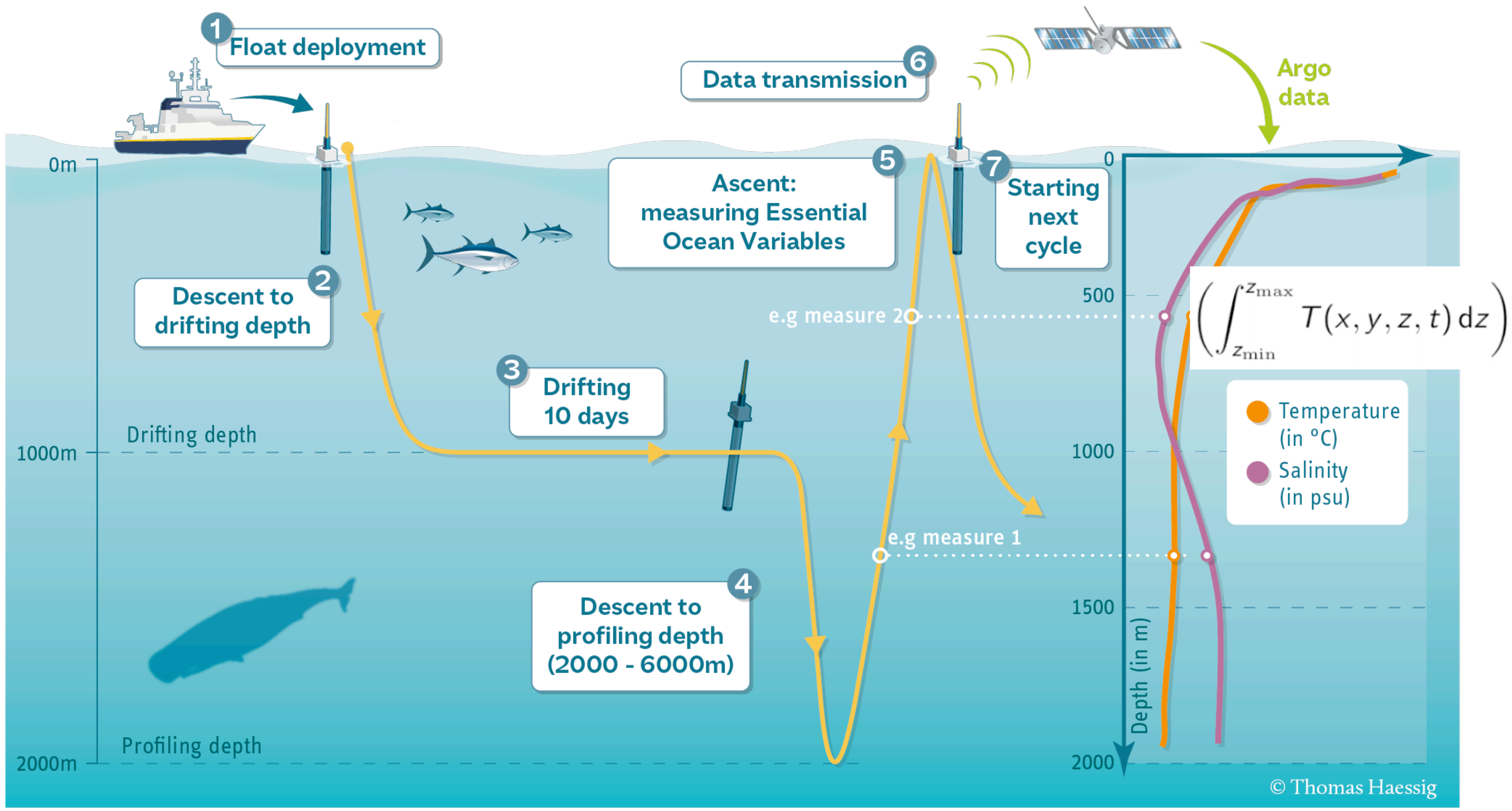
Top layer



Bottom layer

OHC integral must be split into layers due to Argo data availability

$$\mathrm{OHC}(t) = \rho_0 c_{p,0} \int\int \left(\int_{z_{\min}}^{z_{\max}} T(x,y,z,t)\,\mathrm{d}z \right) \mathrm{d}x\,\mathrm{d}y$$



Top layer
(15-975 dbar)

Bottom layer
(975-1850 dbar)